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Ferro- and Antiferroelectric Substances

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## II Data

### Oxides

#### 1 Perovskite-type oxides

##### 1A Simple perovskite-type oxides

##### Nr. 1A-1 $\text{NaNbO}_3$ , Sodium niobate

a	It was reported by MATTHIAS et al. in 1951 that $\text{NaNbO}_3$ was ferroelectric. CROSS et al., however, proved in 1955 that at room temperature it is not ferroelectric but antiferroelectric.					51M2 55C2
b	phase	V	IV	III*	II	I
	state	F	A			P
	crystal system	monoclinic	orthorhombic	pseudo-tetragonal	tetragonal	cubic
	space group		$\text{Pbma}^a$ - $\text{D}_{2h}^{11}$			$\text{Pm3m-O}_h^b$
	$\Theta^{**}$	-200	354	562	640	$^a)61W2$ 58R3
	$P_s \parallel [001]$ in phase V. Phase IV: $a = 5.568 \text{ \AA}$ ( $\cong \sqrt{2}a_0$ ), $b = 5.505 \text{ \AA}$ ( $\cong \sqrt{2}a_0$ ), $c = 15.518 \text{ \AA}$ ( $\cong 4a_0$ ), where $a_0$ is the lattice constant of the cubic cell of phase I. In phase IV (orthorhombic system) the longest edge of a unit cell is taken as the $c$ axis (see Fig. 1). This system of the axes is adopted here. In Well and Megaw's analysis $b$ and $c$ axes were interchanged. The orthorhombic structure is also represented by a pseudomonoclinic unit cell (see Fig. 1), where $b' = c$ , $a' = c'$ ( $\cong a_0$ ), $\beta' \cong \pi/2$ .					51V3 61W2 51W1
2a	Cooling method from a molten mixture of $\text{Na}_2\text{CO}_3$ , $\text{Nb}_2\text{O}_5$ , and $\text{NaF}$ .					
3	Crystal structure: In phase IV, $Z = 8$ . Tab. 1; Fig. 1, 2.					
4	Lattice distortions (thermal expansion): For phase I, II, III, IV: Tab. 2,3; Fig. 3. For phase V, at $-160^\circ\text{C}$ : $a = 5.564 \text{ \AA}$ ( $\cong \sqrt{2}a_0$ ), $b = 5.548 \text{ \AA}$ ( $\cong \sqrt{2}a_0$ ), $c = 7.812 \text{ \AA}$ ( $\cong 2a_0$ ), $\beta = 91^\circ 09'$ . Fig. 4.					57J1
5a	Dielectric constants: Fig. 5. Curie-Weiss law: $\kappa = C/(T - \Theta_p)$ , $T > \Theta_{\text{III-IV}}$ , where $C = 2 \dots 4 \cdot 10^5 \text{ } ^\circ\text{K}$ and $\Theta_p = 60 \dots 80^\circ\text{C}$ .					54S3 55C2
c	Spontaneous polarization: $P_s \cong 12 \cdot 10^{-3} \text{ C m}^{-2}$ ( $\parallel c$ , in phase V). Coercive and critical field for normal and double hysteresis curve: Fig. 6.					
9a	Birefringence: Fig. 7, 8.					55C2, 64p1, 62M9, 62W3
14a	Domain structure: See					
b	Dynamic properties: Fig. 9, 10.					

Tab. 1.  $\text{NaNbO}_3$ . Fractional coordinates  $x, y, z$  of atoms in unit cell at RT. [61W2]

	$x$	$y$	$z$
Na(1)	$\frac{1}{2}$	0.250	0
Na(2)	0.769	0.251	$\frac{1}{2}$
Nb	0.261	0.257	0.125
O(1)	$\frac{1}{2}$	0.208	0
O(2)	0.271	0.290	$\frac{1}{2}$
O(3)	0.010	0.532	0.121
O(4)	0.446	0.972	0.126

- \* According to Ismailzade phase III consists of 4 phases (see Fig. 3). [63I4]  
 \* Transitions exhibit large temperature hysteresis, and the transition temperatures measured with decreasing temperature are given here.

Tab. 2.  $\text{NaNbO}_3$ . Lattice parameters at various temperatures. [56F1] and [54S3]

$T [^\circ\text{C}]$	Crystal symmetry	Lattice parameters	
		[56F1]	[54S3]
20	Monoclinic	$a' = c' = 3.914 \text{ \AA}$ $b' = 4 \cdot 3.881 \text{ \AA}$ $\beta' = 90^\circ 39'$	$a' = c' = 3.915 \text{ \AA}$ $b' = 4 \cdot 3.881 \text{ \AA}$ $\beta' = 90^\circ 40'$
390	Pseudotetragonal	$a = 2 \cdot 3.920 \text{ \AA}$ $c = 4 \cdot 3.926 \text{ \AA}$ $c/a = 2.0032$	$a = 2 \cdot 3.919 \text{ \AA}$ $c = 4 \cdot 3.927 \text{ \AA}$ $c/a = 2.0040$
420	Pseudotetragonal	$a = 2 \cdot 3.924 \text{ \AA}$ $c = 4 \cdot 3.924 \text{ \AA}$ $c/a \approx 2.0000$	$a = 2 \cdot 3.921 \text{ \AA}$ $c = 4 \cdot 3.927 \text{ \AA}$ $c/a = 2.0028$
560	Tetragonal (changing to simple perovskite-type cell)	$a = 2 \cdot 3.933 \text{ \AA}$ $c = 4 \cdot 3.940 \text{ \AA}$ $c/a = 2.0038$	— — —
640	Cubic	$a = 3.942 \text{ \AA}$	—

Tab. 3.  $\text{NaNbO}_3$ . Lattice parameters of the subcell at various temperatures. [63I4]. See Fig. 3

$T [^\circ\text{C}]$	Subcell parameters				
	pseudomonoclinic I ( $a' = c' > b'$ , $\beta' > 90^\circ$ )				
	$a' [\text{\AA}]$	$b' [\text{\AA}]$	$\beta' - 90^\circ$	$a'/b'$	$V [\text{\AA}^3]$
18 ... 20	3.914 <sub>7</sub>	3.885	40'	1.0075 <sub>5</sub>	59.5 <sub>3</sub>
100	3.917 <sub>7</sub>	3.893 <sub>6</sub>	37	1.0060 <sub>5</sub>	59.7 <sub>4</sub>
150	3.919 <sub>5</sub>	3.898 <sub>5</sub>	33	1.0055 <sub>5</sub>	59.9 <sub>4</sub>
200	3.922 <sub>4</sub>	3.902 <sub>6</sub>	29	1.0050 <sub>5</sub>	60.0 <sub>6</sub>
250	3.924 <sub>3</sub>	3.907 <sub>5</sub>	26	1.0040 <sub>5</sub>	60.1 <sub>7</sub>
300	3.925 <sub>4</sub>	3.914 <sub>4</sub>	22	1.0030 <sub>5</sub>	60.3 <sub>2</sub>
340	3.926 <sub>3</sub>	3.917 <sub>5</sub>	18	1.0025 <sub>5</sub>	60.4 <sub>2</sub>
350	3.926 <sub>5</sub>	3.919 <sub>7</sub>	17	1.0020 <sub>2</sub>	60.4 <sub>2</sub>
pseudomonoclinic II					
360	3.927 <sub>3</sub>	3.920 <sub>7</sub>	6	1.0020 <sub>5</sub>	60.45
380	3.927 <sub>8</sub>	3.921 <sub>3</sub>	5	1.0015 <sub>9</sub>	60.50
400	3.928 <sub>3</sub>	3.922 <sub>3</sub>	4	1.0015 <sub>5</sub>	60.5 <sub>2</sub>
pseudomonoclinic III					
420	3.929 <sub>4</sub>	3.923 <sub>7</sub>	3	1.0015 <sub>5</sub>	60.5 <sub>5</sub>
440	3.930 <sub>7</sub>	3.924 <sub>7</sub>	3	1.0015 <sub>5</sub>	60.60
460	3.932 <sub>7</sub>	3.926 <sub>3</sub>	3	1.0015 <sub>5</sub>	60.70
pseudomonoclinic IV					
480	3.933 <sub>5</sub>	3.927 <sub>5</sub>	3	1.0015 <sub>3</sub>	60.7 <sub>7</sub>
500	3.934 <sub>5</sub>	3.928 <sub>8</sub>	2	1.0015 <sub>5</sub>	60.8 <sub>2</sub>
510	3.935 <sub>5</sub>	3.929 <sub>5</sub>	2	1.0015 <sub>5</sub>	60.85
tetragonal I					
$T [^\circ\text{C}]$	$c [\text{\AA}]$	$a = b [\text{\AA}]$	$c/a$	$V [\text{\AA}^3]$	
520	3.936 <sub>7</sub>	3.929 <sub>5</sub>	1.0015 <sub>9</sub>	60.80	
540	3.938 <sub>7</sub>	3.930 <sub>2</sub>	1.0020 <sub>8</sub>	60.85	
560	3.939 <sub>8</sub>	3.931 <sub>6</sub>	1.0020 <sub>8</sub>	60.90	
tetragonal II					
580	3.941 <sub>4</sub>	3.934 <sub>2</sub>	1.0020 <sub>8</sub>	61.00	
600	3.943 <sub>3</sub>	3.937 <sub>8</sub>	1.0015 <sub>5</sub>	61.15	
620	3.945 <sub>6</sub>	3.942 <sub>7</sub>	1.0010 <sub>5</sub>	61.30	
630	3.945 <sub>7</sub>	$\approx 3.945$	$\approx 1.0000$	61.40	
cubic					
$T [^\circ\text{C}]$	$a_0 [\text{\AA}]$	$V [\text{\AA}^3]$	$T [^\circ\text{C}]$	$a_0 [\text{\AA}]$	$V [\text{\AA}^3]$
640	3.947 <sub>3</sub>	61.50	700	3.949 <sub>7</sub>	61.6 <sub>2</sub>
650	3.947 <sub>6</sub>	61.5 <sub>2</sub>	720	3.950 <sub>6</sub>	61.6 <sub>7</sub>
680	3.949 <sub>7</sub>	61.5 <sub>7</sub>			

Furuhata/Marutake

Nr. 1A-2  $\text{KNbO}_3$ , Potassium niobate

1a	Ferroelectricity in $\text{KNbO}_3$ was first discovered by MATTHIAS in 1949.				49M4
b	phase	IV	III	II	I
	state	F	F	F	P
	crystal system	rhombohedral	orthorhombic	tetragonal	cubic
	space group		$\text{Bmm}2^a\text{-C}_{2v}^{14}$		$\text{Pm}3\text{m-O}_h^1$
	$\theta$	-10	225	435	$^\circ\text{C}$
	$P_s \parallel [001]$ in phase II (along $[001]$ of phase I), $P_s \parallel [001]$ in phase III (along $[110]$ of phase I), $P_s \parallel [111]$ in phase IV (along $[111]$ of phase I). $T_{\text{melt}} = 1050^\circ\text{C}$ $\rho = 4.590 \cdot 10^3 \text{ kg m}^{-3}$ $a = 5.697 \text{ \AA}$ , $b = 3.971 \text{ \AA}$ , $c = 5.720 \text{ \AA}$ at RT. Transparent. Light yellow.				*)63K2   55R3, 58M3 52L1 67K4
2	Flux method ( $\text{K}_2\text{CO}_3$ flux). Phase diagram of $\text{K}_2\text{CO}_3\text{-Nb}_2\text{O}_5$ system; see Pulling method from the $\text{K}_2\text{CO}_3\text{-Nb}_2\text{O}_5$ mixture Crystal form: square plate				51W1 55R3 58M3
3	Crystal structure: $Z = 1$ in phase I, II, IV. $Z = 2$ in phase III. Tab. 4, 5; Fig. 11.				
4	Temperature dependence of lattice parameters: Tab. 6; Fig. 12.				
5	Dielectric constant: Fig. 13, 14. $\kappa = C/(T - \theta_p)$ , $T > \theta_{\text{II-I}}$ , where $C = 2.42 \cdot 10^5 \text{ }^\circ\text{K}$ , $\theta_p = 360^\circ\text{C}$ . Nonlinear dielectric properties: $\xi = -1.62 \cdot 10^9 \text{ J C}^{-4} \text{ m}^5$ , $\zeta = 1.79 \cdot 10^{10} \text{ J C}^{-6} \text{ m}^9$ . Spontaneous polarization and coercive field: Fig. 15. $P_s = 26 \cdot 10^{-2} \text{ C m}^{-2}$ at $T = \theta_p$ .				56T3 56T3  56T3 56T3
6	Transition heat, transition entropy: Tab. 7.				56T3
7	Piezoelectricity: Fig. 16.				
12	NQR: Tab. 8; Fig. 17 ... 20.				

Tab. 4.  $\text{KNbO}_3$ . Atomic positions in fractional coordinates at RT in phase III. [67K4]

Nb	0, 0, 0
K	$0, \frac{1}{2}, \frac{1}{2} + z_K$
O(1)	$0, \frac{1}{2}, z_1$
O(2)	$\frac{1}{4} + x_2, 0, \frac{1}{4} + z_2$
$z_K$	+0.017
$z_1$	+0.021
$z_2$	+0.035
$x_2$	+0.004

Tab. 5.  $\text{KNbO}_3$ . Interatomic distances and bond angles at RT. [67K4]

	*	distance $\text{\AA}$	**	*	angle $^\circ$
Nb-O(1)	(2)	$1.991 \pm 0.001$	O(2)(s)-Nb-O(2)(s)	(1)	$97.4 \pm 1.2$
Nb-O(2)	(2)	$1.863 \pm 0.007$	O(2)(l)-Nb-O(2)(l)	(1)	$83.4 \pm 1.0$
Nb-O(2)	(2)	$2.180 \pm 0.009$	O(2)(s)-Nb-O(2)(l)	(2)	$89.7 \pm 0.5$
K-O(1)	(1)	$2.837 \pm 0.014$	O(1)-Nb-O(2)(s)	(4)	$92.3 \pm 0.6$
K-O(1)	(2)	$2.848 \pm 0.001$	O(1)-Nb-O(2)(l)	(4)	$87.5 \pm 0.6$
K-O(1)	(1)	$2.883 \pm 0.014$	Nb-O(1)-Nb	(1)	$172.8 \pm 0.7$
K-O(2)	(4)	$2.792 \pm 0.008$	Nb-O(2)-Nb	(2)	$168.6 \pm 0.6$
K-O(2)	(4)	$2.873 \pm 0.010$			
O(1)-O(2)	(4)	$2.780 \pm 0.012$			
O(1)-O(2)	(4)	$2.884 \pm 0.012$			
O(2)-O(2)	(1)	$2.802 \pm 0.024$			
O(2)-O(2)	(1)	$2.894 \pm 0.024$			
O(2)-O(2)	(2)	$2.860 \pm 0.001$			

\* Numbers in this column indicate numbers of equal bonds or angles per formula unit.

\* For the O-Nb-O angles, the letter s or l indicates whether the Nb-O(2) bond involved is short or long.

Tab. 6.  $\text{KNbO}_3$ . Lattice constants and volume of unit cell at various temperatures. [54S3].  $a'$ ,  $c'$ : lattice parameters of pseudotetragonal cell

$T$ °C	$a' = c'$ Å	$b$ Å	$b/a$	$\beta$	$V$ Å <sup>3</sup>
25	4.0375	3.9711	1.0167	90° 15'	64.73
125	4.0374	3.9797	1.0145	90° 15'	64.87
185	4.0363	3.9830	1.0134	90° 13'	64.89
205	4.0369	3.9839	1.0133	90° 14'	64.93
	$a = b$	$c$	$c/a$		
220	3.9972	4.0636	1.0166		64.92
230	3.9978	4.0640	1.0166		64.95
270	3.9992	4.0647	1.0164		65.01
320	4.0023	4.0639	1.0154		65.10
375	4.0048	4.0620	1.0143		65.15
410	4.0080	4.0567	1.0122		65.18
425	4.0214				65.03
450	4.0225				65.09
510	4.0252				65.22

Tab. 7.  $\text{KNbO}_3$ . Transition heat and transition entropy per mole. [54S1]

Transition	$\Delta Q_m$ cal mol <sup>-1</sup>	$\Delta S_m$ cal °K <sup>-1</sup> mol <sup>-1</sup>
IV → III	32	0.12
III → II	85	0.17
II → I	190	0.28
	134	—

Tab. 8.  $\text{KNbO}_3$ . NQR spectrum. [54C1]. The measured frequency ratios intersect the calculated ratios in a straight line at constant  $\eta = 0.806 \pm 0.002$ .  $\eta$  = asymmetry parameter

Crystal structure	$f$ MHz	Measured ratio	Calculated ratio ( $\eta = 0.806$ )	Identification	$e^2qQ/h$ MHz
orthorhombic (20 °C)	3.648				$23.120 \pm 0.05$
	3.030	1.204	1.204	(9/2, 7/2)	
	2.527	1.198	1.196	(3/2, 1/2)	
	2.085	1.214	1.213	(7/2, 5/2)	
rhombohedral (-196 °C)	2.674		( $\eta = 0.0$ )		$16.0 \pm 0.1$
	2.004	1.335	1.333	(9/2, 7/2)	
	1.335	1.503	1.500	(7/2, 5/2)	
				(5/2, 3/2)	

Nr. 1A-3  $\text{NaTaO}_3$ , Sodium tantalate

1a	It was reported by MATTHIAS in 1949 that $\text{NaTaO}_3$ is ferroelectric below 480 °C. No anomalies of the dielectric constants, however, were observed by SMOLENSKII et al.					49M1 57S3
b	phase	IV	III	II	I	57K1 57K1 62I4 51V2
	state	(F)				
	crystal system	orthorhombic	orthorhombic	tetragonal	cubic	
	space group	$\text{Pc}2_1\text{n-C}_{2v}^2$				
$\Theta$		480	550	630	°C	
$a = 5.4941 \text{ Å}$ , $b = 7.7508 \text{ Å}$ , $c = 5.5130 \text{ Å}$ at RT. The cubic cell in phase I becomes pseudomonoclinic in phase IV. Relation between the orthorhombic unit cell and the pseudomonoclinic cell: Fig. 21.						
3	Crystal structure: $Z = 4$ . Atomic positions: Tab. 9; Fig. 22.					
4	Temperature dependence of lattice parameters: Tab. 10; Fig. 23.					

Tab. 9. NaTaO<sub>3</sub>. Fractional coordinates of atoms in the unit cell. [57K1]

Na	$x$ :	$0 - 0.01$	$0 + 0.01$	$\frac{1}{2} - 0.01$	$\frac{1}{2} + 0.01$
	$y$ :	$\frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$
	$z$ :	$0 + 0.02$	$0 - 0.02$	$\frac{1}{2} - 0.02$	$\frac{1}{2} + 0.02$
Ta*	$x$ :	$\frac{1}{2}$	$\frac{1}{2}$	0	0
	$y$ :	0	$\frac{1}{2}$	$\frac{1}{2}$	0
	$z$ :	0	0	$\frac{1}{2}$	$\frac{1}{2}$
O(1)	$x$ :	$0 - 0.02$	$0 + 0.02$	$\frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$
	$y$ :	$\frac{1}{4} + 0.01$	$\frac{1}{4} + 0.01$	$\frac{1}{4} + 0.01$	$\frac{1}{4} + 0.01$
	$z$ :	$\frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$	$0 + 0.02$	$0 - 0.02$
O(2)	$x$ :	$\frac{1}{4} + 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} + 0.04$
	$y$ :	$0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$
	$z$ :	$\frac{1}{4} + 0.04$	$\frac{3}{4} + 0.04$	$\frac{3}{4} - 0.04$	$\frac{1}{4} - 0.04$
O(3)	$x$ :	$\frac{1}{4} + 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} + 0.04$
	$y$ :	$\frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$0 + 0.06$	$0 + 0.06$
	$z$ :	$\frac{1}{4} + 0.04$	$\frac{3}{4} + 0.04$	$\frac{3}{4} - 0.04$	$\frac{1}{4} - 0.04$

Tab. 10. NaTaO<sub>3</sub>. Temperature dependence of the pseudo-cell parameters. [62I4].  
For the notations, see Fig. 21

$T$ [°C]	23	100	200	300	400	450	480	500	550	580	600
$a' = c'$ [Å]	3.889 <sub>5</sub>	3.893 <sub>6</sub>	3.899 <sub>5</sub>	3.907	3.912 <sub>8</sub>	3.916	3.918	3.920	3.923	3.925 <sub>2</sub>	3.927
$b'$ [Å]	3.885 <sub>5</sub>	3.890 <sub>5</sub>	3.896 <sub>5</sub>	3.903 <sub>8</sub>	3.910 <sub>2</sub>	3.913 <sub>6</sub>	3.915 <sub>8</sub>	3.918	3.923	≈3.925 <sub>2</sub>	≈3.927
$\beta - 90^\circ$	22'00"	16'00"	9'00"	6'00"	4'00"	3'30"	2'00"	≈2'00"	1'30"	0'00"	0'00"
$a'/b'$	1.0010	1.0009	1.0009	1.0008	1.0006	1.0006	1.0005	1.0005	1.000	1.000	1.000
$V$ [Å <sup>3</sup> ]	58.8 <sub>0</sub>	59.0 <sub>0</sub>	59.2 <sub>5</sub>	59.5 <sub>5</sub>	59.8 <sub>5</sub>	60.0 <sub>0</sub>	60.1 <sub>0</sub>	60.2 <sub>0</sub>	60.3 <sub>5</sub>	60.4 <sub>5</sub>	60.5 <sub>5</sub>

  

$T$ [°C]	630	660	680
$b = a = c$ [Å]	3.929	3.931	3.932 <sub>5</sub>
$V$ [Å <sup>3</sup> ]	60.6 <sub>5</sub>	60.7 <sub>5</sub>	60.8 <sub>0</sub>

Nr. 1A-4 KTaO<sub>3</sub>, Potassium tantalate

1a	Ferroelectric activity was first reported by MATTHIAS in 1949; <sup>a)</sup> however, recent studies by WEMPLE have proved that the ferroelectric transition does not occur, at least above 1.6 °K. <sup>b)</sup>	<sup>a)</sup> 49M1, 49M4 <sup>b)</sup> 64W2, 65W2
b	KTaO <sub>3</sub> is cubic and its space group is Pm3m-O <sub>h</sub> .  $T_{\text{melt}} = (1357 \pm 3)^\circ\text{C}$ . $\rho = 6.97 \cdot 10^3 \text{ kg m}^{-3}$ . $a = 3.9885 \text{ Å}$ at RT. Transparent, colorless or pale blue (blue in oxygen-deficient crystals). Cleavage: along (100) planes. Hardness: nearly the same as quartz.	64W2, 65W2, 51V2 55R2, 56R2 58R1 51V2 64W2
2a	Flux method: KF flux, <sup>a)</sup> dark small crystals; K <sub>2</sub> CO <sub>3</sub> flux, <sup>b)</sup> large (≈10 mm) transparent crystals. Czochralski-Kyropoulos method: large (≈10 mm) good quality crystals.  Floating technique: planar single crystals. Phase diagram of system K <sub>2</sub> CO <sub>3</sub> -Ta <sub>2</sub> O <sub>5</sub> : Fig. 24. Hydrothermal phase diagram K <sub>2</sub> O-Ta <sub>2</sub> O <sub>5</sub> -H <sub>2</sub> O at 400 °C:	<sup>a)</sup> 62T5, 64W2 <sup>b)</sup> 66U1 64W2, 65W2, 67B7 66W8 67M2
3	$Z = 1$ Crystal structure: cubic perovskite type, (Pm3m-O <sub>h</sub> ). K at 1a position; Ta at 1b position; 3O at 3c position.	51V1, 51V2

\* All positions  $\pm 0.002$ .

**Figuren S. 221 ff.**

[illegible]

Tab.  
modes  
The  
soft r  
—  
 $T [^{\circ}]$

12  
12€  
23€  
29€  
46€

12a	NMR of $^{181}\text{Ta}$ in $\text{KTaO}_3$ : spin-lattice relaxation time, $T_1 \approx 10^{-3}$ sec at RT; spin-spin relaxation time, $T_2 \approx 10^{-5}$ sec at RT; nuclear magnetic moment of $^{181}\text{Ta}$ ( $I = 7/2$ ): $p_n = (2.340 \pm 0.001) \mu_n$ (uncorrected); ( $p_n = (2.35 \pm 0.01) \mu_n$ , after estimated corrections). Nuclear magnetic acoustic resonance: the absorption data were given for $\Delta m = \pm 2$ transition of $^{181}\text{Ta}$ as a function of the angle between magnetic field and sound axis [100].	60B2 67M4 66U1 64W2 67H3 67H3 63W5, 64W2 67H3, 65H2 64W2															
b	ESR of $\text{Eu}^{2+}$ and $\text{Gd}^{3+}$ in $\text{KTaO}_3$ : Tab. 14. ESR of $\text{Fe}^{3+}$ : $g = 1.99 \pm 0.01$ ; $ a  = (345 \pm 10) \cdot 10^{-2} \text{ m}^{-1}$ at 4.2 °K; $a = (288 \pm 5) \cdot 10^{-2} \text{ m}^{-1}$ at RT ( $\text{Fe}^{3+}$ is on the $\text{Ta}^{5+}$ site). $a = (30 \pm 1) \cdot 10^{-2} \text{ m}^{-1}$ at RT ( $\text{Fe}^{3+}$ is on the $\text{K}^{1+}$ site). ESR Stark effect for $\text{Fe}^{3+}$ : $E_{\text{bias}}$ along [100] induces axial splitting term $D$ ( $D = 12 \cdot 10^{-2} \text{ m}^{-1}$ at $E_{\text{bias}} = 1.0 \text{ MV m}^{-1}$ at 4.2 °K; $D \propto E_{\text{bias}}^2$ ). ESR of $\text{Ni}^{3+}$ located on $\text{Ta}^{5+}$ site (low spin state) and on $\text{K}^{1+}$ site: see ESR in Mn-doped, Co-doped and Cr-doped $\text{KTaO}_3$ : see																
13b	Phonon dispersion relation for the transverse optical branch: Fig. 52; Tab. 15. Temperature dependence of the ferroelectric soft mode: Fig. 53. The square of the phonon energy of the ferroelectric soft mode can be approximated by $(\hbar\nu)^2 = 10^4 A/\kappa$ , $40^\circ\text{K} < T < 295^\circ\text{K}$ ; where $A = 2.825 (\text{meV})^2$ , $\kappa(T)$ is the dielectric constant. For the ferroelectric soft mode, see also 1A-4-9a. Phonon energies of the acoustic modes: Fig. 54.	67S11 67S11															
17	Etchant: single crystal is slowly etched by dilute HF. Band structure and the related properties: see references; also 1A-4-9a, 9b, 9d, 10, and Tab. 12. Band gap energies determined by various methods:	64W2 67F4, 67B1															
<table border="1"> <thead> <tr> <th>Method</th><th>296 °K</th><th>77 °K</th></tr> </thead> <tbody> <tr> <td>Faraday rotation</td><td>3.77 eV 3.62 eV</td><td>3.79 eV 3.65 eV</td></tr> <tr> <td>Electroreflectance singularities</td><td>3.57 eV 3.80 eV</td><td></td></tr> <tr> <td>Absorption data</td><td>3.75 eV</td><td></td></tr> <tr> <td>Energy at which <math>\alpha \approx 10^6 \text{ m}^{-1}</math></td><td>3.79 eV</td><td></td></tr> </tbody> </table>		Method	296 °K	77 °K	Faraday rotation	3.77 eV 3.62 eV	3.79 eV 3.65 eV	Electroreflectance singularities	3.57 eV 3.80 eV		Absorption data	3.75 eV		Energy at which $\alpha \approx 10^6 \text{ m}^{-1}$	3.79 eV		67B1
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Energy at which $\alpha \approx 10^6 \text{ m}^{-1}$	3.79 eV																
Cyclotron resonance of semiconducting $\text{KTaO}_3$ at 70 GHz and 1.4 °K: microwave skin depth, about 30 $\mu\text{m}$ ; see reference paper for the microwave absorption vs. magnetic field curves.		65S13															

Tab. 11.  $\text{KTaO}_3$ . Transverse optical modes at various temperatures [67P4]. The wave number  $\tilde{\nu}_{11}$  (ferroelectric soft mode) is temperature dependent.

$T [^\circ\text{K}]$	$\tilde{\nu}_{11}$	$\tilde{\nu}_{12}$	$\tilde{\nu}_{13}$
	$\cdot 10^3 \text{ m}^{-1}$		
12	25	196	—
126	58	198	551
232	79	198	551
295	88	199	550
463	106	199	—

Tab. 12.  $\text{KTaO}_3$ . (Ca-doped). Singularities observed in electroreflectance spectra (in eV) [67F4]. See Figs. 40, 41

	$E_1$	$E_2$	$A_1$	$A'_1$	$A_2$
	[eV]				
$\text{KTaO}_3$ (100)	3.57	3.80	4.40	4.88	5.50
$\text{KTaO}_3$ (111)	—	3.77	4.45	4.90	5.47
$\text{KTaO}_3$ (110)	3.55	3.80	4.47	4.85	5.50

Tab. 13.  $\text{KTaO}_3$  (reduced). Hall coefficient  $R_H$  and Hall mobility  $\mu_H$  at 295 °K and 4.2 °K for single crystals [65W2]. Carrier concentrations  $N$  are calculated from the 4.2 °K Hall coefficient using  $R_H = -1/Ne$

Sample Nr.	$N_{\text{calc}} \text{ m}^{-3}$	$R_H \text{ m}^3 \text{ C}^{-1}$		$\mu_H \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	
		(295°K)	(4.2°K)	(295°K)	(4.2°K)
1	$3.5 \cdot 10^{23}$	$20.3 \cdot 10^{-6}$	$18 \cdot 10^{-6}$	$2.7 \cdot 10^{-3}$	2.3
2	$6.0 \cdot 10^{23}$	$12.9 \cdot 10^{-6}$	$10.4 \cdot 10^{-6}$	$2.9 \cdot 10^{-3}$	1.9
3	$6.6 \cdot 10^{23}$	$11.5 \cdot 10^{-6}$	$9.4 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	1.9
4	$2.4 \cdot 10^{24}$	$3.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	1.1
5	$7.8 \cdot 10^{24}$	$1.0 \cdot 10^{-6}$	$0.80 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	0.53
6	$1.3 \cdot 10^{25}$	$0.62 \cdot 10^{-6}$	$0.48 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	0.34



Tab. 14.  $\text{KTaO}_3$ . Parameters of ESR spectrum of  $\text{Eu}^{2+}$  and  $\text{Gd}^{3+}$  ions, doped in single crystals of  $\text{KTaO}_3$  [66U1]

Tab. 14. $\text{KTaO}_3$ . Parameters of $\text{Eu}^{2+}$ and $\text{Gd}^{3+}$ in $\text{KTaO}_3$ [6607]									
Para-magnetic center	Site	S	$\mathcal{K}$	$\nu$ GHz	T °K	g-factor	FS	HFS	
							$b_{40}, b_{60}$ $10^{-2} \text{ m}^{-1}$	I	A $10^{-2} \text{ m}^{-1}$
$\text{Eu}^{2+}$	$\text{K}^+$	7/2	(8)	9.1	77	$1.990 \pm 0.002$	$b_{40} = (\pm)16 \pm 2$ $b_{60} = (\pm)1.2 \pm 0.6$	5/2 5/2	$ ^{151}\text{A}  = 36 \pm 1$ $ ^{153}\text{A}  = 16 \pm 1$
$\text{Gd}^{3+}$		7/2			4.2	$1.990 \pm 0.002$	$b_{40} = -8.14 \pm 0.27$ $b_{60} = +0.47 \pm 0.3$		
					77	$1.990 \pm 0.002$	$b_{40} = -7.0 \pm 0.3$ $b_{60} = +0.5 \pm 0.5$		

Tab. 15.  $\text{KTaO}_3$ . Phonon energies of the soft ferroelectric mode (transverse optical mode) at various temperatures [67S11]. The wave vector  $q$  at the zone boundary is  $0.788 \text{ \AA}^{-1}$  ( $=\pi/a$ ). See Fig. 52

T °K	Phonon energy [meV] for $q [\text{\AA}^{-1}] =$		
	0	0.1	0.2
295	10.7	11.5	13.5
230	9.7		
170	8.6	10.0	12.5
120	7.3		
77	5.7	7.5	10.7
40	4.2	6.0	
28	3.6	5.9	10.5
15	3.0	5.3	
10	3.2	5.2	
4	3.1	5.3	9.8

Nr. 1A-5  $\text{CaTiO}_3$ , Calcium titanate (Perovskite)Tab. 16.  $\text{CaTiO}_3$ . Ion positions. [57K2]

4 Ti in 4(a):	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0; 0, \frac{1}{2}, \frac{1}{2}$
4 Ca in 4(c):	$x, \frac{1}{2}, z; \bar{x}, \frac{1}{2}, \bar{z}; \frac{1}{2} + x, \frac{1}{2}, \frac{1}{2} - z; \frac{1}{2} - x, \frac{1}{2}, \frac{1}{2} + z;$ with $x = 0, z = 0.030$ .
4 O in 4(c):	with $x = \frac{1}{2} - 0.037, z = -0.018$ .
8 O in 8(d):	$x, y, z; \frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z;$ $\bar{x}, \frac{1}{2} + y, \bar{z}; \frac{1}{2} + x, \bar{y}, \frac{1}{2} - z;$ $\bar{x}, \bar{y}, \bar{z}; \frac{1}{2} + x, \frac{1}{2} + y, \frac{1}{2} - z;$ $x, \frac{1}{2} - y, z; \frac{1}{2} - x, y, \frac{1}{2} + z;$ with $x = \frac{1}{4} - 0.018, y = -0.026, z = \frac{1}{4} - 0.018$ .

1a Specific heat anomaly associated with a phase transition was observed in  $\text{CaTiO}_3$  at about 1260 °C by NAYLOR et al. in 1946. GRÄNICHNER et al. reported that  $\text{CaTiO}_3$  becomes cubic above 1260 °C.

b phase	II	I
state		P
crystal system	orthorhombic	cubic
space group	$\text{Pcmn-D}_{2h}^{16}$	

$\Theta \approx 1260 \text{ °C}$

$\rho = 4.10 \cdot 10^3 \text{ kg m}^{-3}$  at RT.  
 $T_{\text{melt}} = 1960 \text{ °C}$

$a = 5.3670 \text{ \AA}, b = 7.6438 \text{ \AA}, c = 5.4439 \text{ \AA}$  at RT.

The ideal perovskite cubic unit cell becomes pseudo-monoclinic in phase II in the same manner as shown in Fig. 21.  $\beta' = 90^\circ 48'$  at RT.

Transparent, colorless.

2 Flux method; flux:  $\text{CaCl}_2, \text{BaCl}_2, \text{CaCl}_2 + \text{BaCl}_2, \text{Na}_2\text{CO}_3 + \text{K}_2\text{CO}_3$ .  
Flame fusion method:

3 Crystal structure:  $Z = 4$  in phase II.  
Fig. 55; Tab. 16.

4 Lattice distortion: Fig. 56.

5a Dielectric constant:  $\kappa = 186, \tan \delta = 3 \cdot 10^{-4}$  at RT.  
Fig. 57.

6a Specific heat: Fig. 58.  
Transition heat:  $\Delta Q = 550 \text{ cal mol}^{-1}$  at  $\Theta_{\text{II-I}}$ .

46N1, 54G1

54G1

57K2

46N1

62M3

62M3

57K2

57K2

58L1, 62M3

57K2

62M3

46N1

9a	Nr. 1A-5 CaTiO <sub>3</sub> continued Refractive indices: Fig. 59. Reflection and absorption: Fig. 60, 61.			
17	Hardness: Mohs 6.5 ... 7, Knoop 986			62M3
Nr. 1A-6 SrTiO <sub>3</sub> , Strontium titanate				
1a	Ferroelectric-like behavior of SrTiO <sub>3</sub> was first observed by GRÄNICHER in 1956.			56G2
b	phase	II*	I	62R1
	state	(F)	P	
	crystal system	tetragonal	cubic**	
	space group		Pm3m-O <sub>h</sub> <sup>1</sup>	
	Θ	110	°K	
	$T_{\text{melt}} \cong 2000$ °C. $\rho = 5.11 \cdot 10^3$ kg m <sup>-3</sup> . $a = 3.905$ Å at RT. Transparent, colorless			63f2, 64L1 63f2 64L4
2a	Crystal growth: Flux method (flux: KF or 50% Na <sub>2</sub> CO <sub>3</sub> + 50% K <sub>2</sub> CO <sub>3</sub> ). Flame-fusion (Verneuil) method. Phase diagram of the system SrO-TiO <sub>2</sub> is given in Figs. 297 and 289 of [64L1].			57N1 61G1 64L1
3	Crystal structure: $Z = 1$ . Fig. 62.			
4	Thermal expansion: Fig. 63.			
5a	Dielectric constant: Figs. 64 ... 76. Expression of $\kappa$ vs. $T$ curve: Curie-Weiss law: $\kappa = C/(T - \Theta_p)$ , $T > 70$ °K, where $C = 7.83 \cdot 10^4$ °K, $\Theta_p = 28$ °K, $\kappa = M/[(T_1/2) \coth(T_1/2T) - T_0]$ , $T < 50$ °K, where $T_0 = 38$ °K, $T_1 = 84$ °K, $M = 9 \cdot 10^4$ °K.			61M3 59W2, 62S2
b	Coefficients of free energy expansion at low temperatures:			66C6
c	Saturation polarization: Fig. 77. Remanent polarization: Fig. 78.			
d	Electrocaloric effect: Fig. 79. For additional data, see			64K5, 65H4, 61H1
6a	Specific heat: Fig. 80. Specific heat below 1 °K, see			61g1, 66A4
b	Thermal conductivity: Figs. 81, 82. For ceramics: see also			58Y1, 60Y1, 61g1, 66H9
7a	Piezoelectricity (dc bias induced piezoelectricity): Figs. 83, 84, 85.			
b	Electrostriction: Fig. 86.			
8a	Elastic compliances and stiffnesses: Tab. 17; Figs. 87, 88, 89.			
9a	Refractive indices: Tabs. 18, 19; Fig. 90. Reflectivity, absorption coefficient and dielectric constant: (i) Infrared region: Figs. 91 ... 95. See also Tab. 42. (ii) Visible and ultraviolet region: Figs. 96 ... 102. See also Tab. 43.			
b	Quadratic electrooptic effect: $M_{11} - M_{12} = (0.14 \pm 0.01) \text{ m}^4 \text{ C}^{-2}$ at 6328 Å (4.2 ... 300 °K).			64G3
c	Piezooptic effect: Tabs. 20, 21.			
* In phase II a hysteresis loop is observed, a), b) but the remanent polarization depends upon the amplitude of the applied field. According to LYTLE, phase II consists of three phases. a) [59W2], b) [61M3], [64L4]				
** Generally the phase I is believed to be cubic but evidence of pseudo-cubic structure was reported by a few authors. [64L4], [66C6]				

9d	Nr. 1A-6 SrTiO <sub>3</sub> continued	67B1
e	Faraday rotation: Fig. 103. See also Tab. 44. Raman effect: Fig. 104. Brillouin scattering: Fig. 105. See	66K1
10	Electrical resistivity: $\rho > 10^7 \Omega \text{m}$ (good quality single crystal) at RT. Fig. 106. For additional data, see Tab. 22. Resistivity, Hall coefficient and Hall mobility of semiconductive samples: Tab. 23; Figs. 107 ... 110. For additional data, see Hall mobility for photo-excited electron: see Fig. 115. Piezoresistivity: Figs. 111, 112, 113. Photoconductivity: Figs. 114, 115. Photoemission: Fig. 116. Superconductivity: discovered in semiconductive SrTiO <sub>3</sub> by SCHOOLEY et al. in 1964. Figs. 117 ... 120. Tab. 24. Penetration depth of static magnetic field in superconductive SrTiO <sub>3</sub> is of the order of $10^{-5} \text{ m}$ .	61g1 61g1  64F5, 67T6 66T10  64S5 66S16
11	Magnetic susceptibility: Tab. 25.	
12a	NMR: Fig. 121.	
b	ESR: Tab. 26; Figs. 122 ... 130.	
c	Mössbauer effect: Figs. 131, 132.	
13c	Inelastic neutron scattering: Tab. 27; Figs. 133, 134, 135.	
14a	Domain structure: A fine twin structure was observed in phase II. The appearance of the twin structure is similar to that of the 90° domains in tetragonal BaTiO <sub>3</sub> . The dc field, however, does not change the twin structure.	61M3, 64L4
16	Radiation damage: Fig. 136.	66R6
17	Etching and chemical polishing: Band structure and related properties: The band structure was determined theoretically by KAHN et al: Fig. 137. For discussions, see Magnetoresistance, Shubnikov-deHaas effect. The conduction band consists of spheroids along [100] having 3 minima at $X_3$ . The transverse and longitudinal effective electron mass: $m_t = 1.5 m_0 (\pm 15\%)$ , $m_l = 6.0 m_0 (\pm 30\%)$ .	64K1 65S18 66F3, 67F3 67F3

Tab. 17. SrTiO<sub>3</sub>. Elastic constants at RT

$s_{11}$	$s_{12}$	$s_{13}$	$c_{11}$	$c_{12}$	$c_{13}$	Method	Note	Reference
$10^{-12} \text{ m}^2 \text{ N}^{-1}$			$10^{11} \text{ N m}^{-2}$					
3.3	-0.74	8.4	3.48	1.01	1.19	composite-bar	$c$ calculated from $s$	58p5
3.729	-0.909	8.091	3.181	1.025	1.236	pulse	$s$ calculated from $c$	63B2
3.772 $\pm 0.023$	-0.926 $\pm 0.010$	8.233 $\pm 0.040$	3.156 $\pm 0.027$	1.027 $\pm 0.027$	1.215 $\pm 0.006$	pulse	$s$ calculated from $c$	63W1

Tab. 18. SrTiO<sub>3</sub>.  $n$  vs.  $\lambda$  at 21 °C. [57G1]

$\lambda$ Å	$n$	$\lambda$ Å	$n$	$\lambda$ Å	$n$
4200	2.6050	5400	2.4386	6600	2.3771
4300	2.5810	5500	2.4312	6700	2.3737
4400	2.5585	5600	2.4245	6800	2.3703
4500	2.5394	5700	2.4182	6900	2.3674
4600	2.5236	5800	2.4122	7000	2.3645
4700	2.5101	5900	2.4069	7100	2.3617
4800	2.4970	6000	2.4019	7200	2.3590
4900	2.4846	6100	2.3971	7300	2.3564
5000	2.4734	6200	2.3928	7400	2.3538
5100	2.4636	6300	2.3886	7500	2.3514
5200	2.4548	6400	2.3846	7600	2.3490
5300	2.4464	6500	2.3807	7700	2.3468

Tab. 19. SrTiO<sub>3</sub>.  $n$  vs.  $\lambda$  [65B9]

$\lambda$ μm	$n$	$\lambda$ μm	$n$
0.45	2.537	1.8	2.270
0.5	2.472	2.0	2.264
0.6	2.402	2.2	2.258
0.7	2.363	2.4	2.2524
0.8	2.340	2.6	2.2490
0.9	2.326	2.8	2.2395
1.0	2.315	3.0	2.2315
1.1	2.306	3.2	2.2236
1.2	2.299	3.4	2.2143
1.4	2.287	3.6	2.2058
1.6	2.279	3.8	2.1951

Tab. 20.  $\text{SrTiO}_3$ .  $\Pi_{66}$  vs.  $\lambda$  at  $(27 \pm 1)^\circ\text{C}$ . [57Gf]

$\lambda$ Å	$\Pi_{66}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$	$\lambda$ Å	$\Pi_{66}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$
4200	-3.69	6000	-4.92
4300	-3.74	6100	-4.99
4400	-3.78	6200	-5.05
4500	-3.99	6300	-5.12
4600	-3.965	6400	-5.13
4700	-4.13	6500	-5.18
4800	-4.09	6600	-5.22
4900	-4.22	6700	-5.29
5000	-4.33	6800	-5.52
5100	-4.32	6900	-5.48
5200	-4.41	7000	-5.555
5300	-4.51	7100	-5.62
5400	-4.59	7200	-5.77
5500	-4.575	7300	-5.73
5600	-4.62	7400	-5.78
5700	-4.69	7500	-5.79
5800	-4.79	7600	-5.825
5900	-4.85	7700	-5.98

Tab. 21.  $\text{SrTiO}_3$ .  $\Pi_{21} - \Pi_{11}$  vs.  $\lambda$  at  $(27 \pm 1)^\circ\text{C}$ . [57Gf]

$\lambda$ Å	$\Pi_{21} - \Pi_{11}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$	$\lambda$ Å	$\Pi_{21} - \Pi_{11}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$
4200	9.03	6000	9.95
4300	9.23	6100	9.94
4400	9.03	6200	9.91
4500	9.26	6300	9.84
4600	9.12	6400	9.82
4700	9.12	6500	9.88
4800	9.14	6600	9.96
4900	9.16	6700	9.92
5000	9.35	6800	9.98
5100	9.44	6900	9.99
5200	9.61	7000	9.91
5300	9.54	7100	9.92
5400	9.68	7200	9.94
5500	9.56	7300	9.99
5600	9.85	7400	10.05
5700	9.85	7500	9.90
5800	9.86	7600	9.92
5900	9.88	7700	10.02

Tab. 22.  $\text{SrTiO}_3$  (single crystal). Effects of electrode material on the apparent conductivity [65C6]. Measurements were made by the two terminal method at  $T = 130^\circ\text{C}$ ,  $t = 24$  hours after the application of the field  $E = 100 \text{ kV m}^{-1}$ 

Electrode material	$\sigma$ [ $\Omega^{-1} \text{ m}^{-1}$ ] after 24 h at $130^\circ\text{C}$	Form of $\sigma$ vs. $t$ curve
Au	$4.8 \cdot 10^{-7}$	Fall then rise
Ag	$8.8 \cdot 10^{-8}$	As for gold
Sn	$8.8 \cdot 10^{-9}$	Fall followed by slow rise but without saturation
Cr	$6.0 \cdot 10^{-11}$	Continuous fall tending toward steady value
Cd	$9.5 \cdot 10^{-11}$	Similar to chromium
Al	$2.9 \cdot 10^{-10}$	Similar to chromium (for a field of $400 \text{ kV m}^{-1}$ behavior is like that of gold)

Tab. 23.  $\text{SrTiO}_3$  (single crystal). The  $300^\circ\text{K}$  and  $2^\circ\text{K}$  Hall coefficient  $R_H$  and Hall mobility  $\mu_H$  values and the  $300^\circ\text{K}$  electron concentrations for semiconductive single crystals. [67T6]. In the first column, (Nb) means Nb-doped samples, the other samples are reduced ones

Sample	$300^\circ\text{K}$		$2^\circ\text{K}$		$n = \frac{1}{eR_H(300^\circ\text{K})}$ $\text{m}^{-3}$
	$R_H$ $10^{-6} \text{ m}^3 \text{ C}^{-1}$	$\mu_H$ $10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	$R_H$ $10^{-6} \text{ m}^3 \text{ C}^{-1}$	$\mu_H$ $10^{-1} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	
5	0.26	6.5	0.25	1.0	$2.4 \cdot 10^{25}$
2	0.62	5.2	0.77	1.8	$1.0 \cdot 10^{25}$
3	1.8	7.2	3.9	2.7	$3.5 \cdot 10^{24}$
6	5.3	8.0	11.0	3.1	$1.2 \cdot 10^{24}$
12	14.0	8.0			$4.5 \cdot 10^{23}$
9	23.0	5.8			$2.7 \cdot 10^{23}$
13(Nb)	0.22	5.5	0.22	3.3	$2.8 \cdot 10^{25}$
8(Nb)	0.58	4.8	0.63	8.2	$1.1 \cdot 10^{25}$
10(Nb)	3.4	6.2	3.3	12.0	$1.8 \cdot 10^{24}$
14(Nb)	14.0	6.7	11.0	13.0	$4.5 \cdot 10^{23}$
15(Nb)	22.0	5.4	18.0	19.0	$2.8 \cdot 10^{23}$
11(Nb)	44.0	6.0	33.0	22.0	$1.4 \cdot 10^{23}$

Tab. 24 see page 50

Tab. 25.  $\text{SrTiO}_3$ . Susceptibility in pure and reduced single crystals [66F2].  
 $\Delta\chi_{\text{mag}}$  represents the contribution from the charge carriers;  $\Delta\chi_{\text{mag}}$  is obtained by measuring the  
 $N$  = carrier concentration;  $T_{\text{deg}}$  = degeneracy temperature;  $m^*$  = density-of-state effective mass

Sample	$N$ at 4.2 °K $\text{m}^{-3}$	$T_{\text{deg}}$ °K	$\chi_{\text{mag}}$ or $\Delta\chi_{\text{mag}} \cdot 10^{-7} \text{ cm}^3 \text{ g}^{-1}$		$m^*$ at 4.2 °K [ $m_0$ ]
			300 °K	78 °K	
pure	—	—	—	—	—
28 h, 950 °C hydrogen	$6 \cdot 10^{24}$	28	-1.02	-1.00	-0.92
5 h, 1200 °C hydrogen	$7.5 \cdot 10^{25}$	148	+0.037	+0.073	—
(carbon boat)	—	—	+0.270	+0.523	+0.928
reoxidized 18 h, 700 °C,	—	—	—	—	—
air	—	—	-1.016	-1.012	-0.919
27 h, 1370 °C hydrogen	$5.3 \cdot 10^{25}$	550	+1.704	+1.763	+1.719
(carbon boat)	—	—	—	—	—

Tab. 27.  $\text{SrTiO}_3$ . The frequency of the lowest  
transverse optic mode at  $q = 0$  for five differ-  
ent temperatures. [62C4]

$T$ °K	Neutron	Far infrared
90	$1.23 \pm 0.03$	1.2 <sup>a)</sup>
142	$1.72 \pm 0.04$	—
203	$2.24 \pm 0.05$	—
296	$2.73 \pm 0.05$	3.0 <sup>a)</sup>
430	$3.32 \pm 0.07$	2.63 <sup>b)</sup>

<sup>a)</sup> [62B2] <sup>b)</sup> [62S12]

Tab. 26.  $\text{SrTiO}_3$ . Summary of the properties of ESR spectrum in  $\text{SrTiO}_3$  for various doped paramagnetic ions

Para- magnetic center	Site	$S$	$\mathcal{H}$	$\nu$ GHz	$T$ °K	$g$ -factor		FS $D, E, a$ [ $10^{-2} \text{ m}^{-1}$ ]	HFS $I$	Ref.	Liter- ature
						$g_{\parallel}$	$g_{\perp}$				
$\text{Cr}^{3+}$	$\text{Ti}^{4+}$	3/2	(5)	9	80	$1.9788 \pm 0.007$	(isotropic)	$D = 2 \pm 0.3, E = 0$	3/2	<sup>f)</sup>	58M7
					300	$1.9780 \pm 0.007$	(isotropic)	$D = 0, E = 0$			62M6
$\text{Mn}^{2+}$	$\text{Ti}^{4+}$	3/2	(5)	10	77	$1.994 \pm 0.001$	(isotropic)	$D = +1.0, E = 0$	5/2		59M4
					RT	$1.994 \pm 0.001$	(isotropic)	$D = -0.7, E = 0$			
$\text{Fe}^{3+}$	$\text{Ti}^{4+}$	5/2	(7)	9	1.9	$2.004 \pm 0.001$	(isotropic)	$D = +17.9 \pm 1.0, E = 0$			
					4.2	$2.004 \pm 0.001$	(isotropic)	$a = -230 \pm 10, E = 0$			
					77	$2.004 \pm 0.001$	(isotropic)	$D = +16.1 \pm 0.7, E = 0$			
					300	$2.004 \pm 0.001$	(isotropic)	$a = -225.6 \pm 1.9$			
$\text{Ni}^{2+}$	$\text{Ti}^{4+}$	1	(4)	10	80	$2.004 \pm 0.001$	(isotropic)	$D = +7.3 \pm 0.3, E = 0$			59D2
$\text{Ni}^{1+}$ or $\text{Ni}^{3+}$	$\text{Ti}^{4+}$	1/2	(2)	10	20	$2.029 \pm 0.001$	(isotropic)	$a = -220.8 \pm 1.1$			58M8
					80	$2.029 \pm 0.001$	(isotropic)	$D = 1.0, E = 0$			
					203	$2.352 \pm 0.001$	(isotropic)	$a = -197.7 \pm 0.7$			62R3

Para- magnetic center	Site	$S$	$\mathcal{H}$	$\nu$ GHz	$T$ °K	$g$ -factor		FS $D, E, a$ [ $10^{-2} \text{ m}^{-1}$ ]	HFS $I$	Ref.	Liter- ature
						$g_{\parallel}$	$g_{\perp}$				



Tab. 24.  $\text{SrTiO}_3$  (ceramics containing Ba or Ca in mol%). Superconductive properties of  $(\text{Ba}_x\text{Sr}_{1-x})\text{TiO}_3$  and  $(\text{Ca}_x\text{Sr}_{1-x})\text{TiO}_3$  [67S8].  $H_{c1}$  is the point at which the magnetization curve first deviates from linearity;  $H_{c1}(0)$  is the extrapolated value for  $T \rightarrow 0^\circ\text{K}$ .  
 $N$  = Carrier concentration  $\Theta_c$  = superconducting transition temperature

% Ba or Ca	$N$ $10^{25} \text{ m}^{-3}$	$\Theta_c$ $^\circ\text{K}$	$H_{c1}(0)$ Oe	% Ba or Ca	$N$ $10^{25} \text{ m}^{-3}$	$\Theta_c$ $^\circ\text{K}$	$H_{c1}(0)$ Oe
—	2.7	0.18		10.0	4.2	0.25	
—	5.8	0.30	2.8	12.5	4.5	<0.10	
—	6.4	0.25	2.8				
—	1.7	0.10		2.5 (Ca)	5.0	0.32	
—	12.0	0.17		5.0	9.2	0.30	
—	23.0	0.10		7.5	74.0	<0.06	
2.5 (Ba)	6.0	0.52		7.5	8.7	0.43	(3.5) <sup>a)</sup>
2.5	0.3	0.23		7.5	0.2	<0.06	
5.0	6.7	0.50	3.9	7.5	0.6	0.37	
7.5	7.0	0.29		7.5	33.0	<0.07	
7.5	0.05	0.22		7.5	2.0	0.48	
7.5	34.0	0.09		7.5	0.06 <sup>b)</sup>	<0.06	
7.5	0.5	0.25		10.0	9.3	0.39	
7.5	2.3	0.27		20.0	13.0	0.29	
7.5	15.0	0.45		30.0	6.7	0.50	1.9
				30.0	0.6	<0.05	

Nr. 1A-7  $\text{CdTiO}_3$ , Cadmium titanate

1a	CdTiO <sub>3</sub> was reported by SMOLENSKII in 1950 to be ferroelectric below 50 ... 60 °K. In 1950 HULM et al. denied its ferroelectricity but HEGENBARTH supported SMOLENSKII's findings.			50S7, 50H2, 59H4
b	phase	II	I	
	state	(F) <sup>a)</sup>		
	crystal system		orthorhombic <sup>b)</sup>	a)50S7
	space group		Pc2 <sub>1</sub> n <sup>b)</sup> -C <sub>2v</sub> <sup>2</sup>	b)57K1
	Θ	-223... -213 °C		
	Lattice constants: a = 5.348 Å, b = 7.615 Å, c = 5.417 Å at RT. The relation between the orthorhombic unit cell and the pseudo-cubic monoclinic cell is the same as in the case of NaTaO <sub>3</sub> ; see Fig. 21.			50S7 57K1
2	Flux method (flux: 40 wt% NaCl + 40 wt% NaBO <sub>2</sub> + 20 wt% Na <sub>2</sub> CO <sub>3</sub> ).			
3	Z = 4. Crystal structure in phase I: Tab. 28; Fig. 138.			57K1
5a	Dielectric constant: κ = 250 at RT. κ = C/(T - Θ <sub>p</sub> ), C = 4.5 · 10 <sup>4</sup> °K.			
b	Effect of E <sub>bias</sub> on κ: Fig. 139.			50S7, 50H2

Tab. 28.  $\text{CdTiO}_3$ .  
Fractional coordinates of atoms in the unit cell.  
[57K1]

		Positions				Estimated error
Cd	$x$ :	$0 + 0.006$	$0 - 0.006$	$\frac{1}{2} + 0.006$	$\frac{1}{2} - 0.006$	$\pm 0.002$
	$y$ :	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	
	$z$ :	$0 + 0.016$	$0 - 0.016$	$\frac{1}{2} - 0.016$	$\frac{1}{2} + 0.016$	$\pm 0.002$
Ti	$x$ :	$\frac{1}{2} + 0.005$	$\frac{1}{2} - 0.005$	$0 + 0.005$	$0 - 0.005$	$\pm 0.005$
	$y$ :	$0$	$\frac{1}{2}$	$\frac{1}{2}$	$0$	
	$z$ :	$0 - 0.065$	$0 + 0.065$	$\frac{1}{2} + 0.065$	$\frac{1}{2} - 0.065$	$\pm 0.010$
O(1)	$x$ :	$0 - 0.03$	$0 + 0.03$	$\frac{1}{2} + 0.03$	$\frac{1}{2} - 0.03$	$\pm 0.015$
	$y$ :	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{1}{4}$	$\pm 0.025$
	$z$ :	$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$0 + 0.05$	$0 - 0.05$	$\pm 0.015$
O(2)	$x$ :	$\frac{1}{4} + 0.05$	$\frac{1}{4} - 0.05$	$\frac{3}{4} - 0.05$	$\frac{3}{4} + 0.05$	$\pm 0.005$
	$y$ :	$0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$	$\pm 0.015$
	$z$ :	$\frac{1}{4} + 0.06$	$\frac{3}{4} + 0.06$	$\frac{3}{4} - 0.06$	$\frac{1}{4} - 0.06$	$\pm 0.015$
O(3)	$x$ :	$\frac{1}{4} + 0.05$	$\frac{1}{4} - 0.05$	$\frac{3}{4} - 0.05$	$\frac{3}{4} + 0.05$	$\pm 0.005$
	$y$ :	$\frac{1}{2} + 0.07$	$\frac{1}{2} + 0.07$	$0 + 0.07$	$0 + 0.07$	$\pm 0.015$
	$z$ :	$\frac{1}{4} + 0.06$	$\frac{3}{4} + 0.06$	$\frac{3}{4} - 0.06$	$\frac{1}{4} - 0.06$	$\pm 0.015$

<sup>a)</sup> This specimen is not spherical, so that the value of  $H_{c1}(0)$  quoted is only approximate.

<sup>b)</sup> Hall coefficient appeared to be affected by magnetic history of specimen at liquid helium temperature.

Nr. 1A-8 BaTiO<sub>3</sub>, Barium titanate

(Responsible authors for this section are as follows: IKEDA, NAKAMURA, NOMURA, SAWAGUCHI, SHIOZAKI and TOYODA, abbreviated as INaNoSaShiTo).

1a	The anomalous dielectric properties of BaTiO <sub>3</sub> were discovered on ceramic specimens independently by WAINER and SOLOMON in 1942, by OGAWA in 1944 and by WUL in 1945. The ferroelectric activity of BaTiO <sub>3</sub> was reported independently by VON HIPPEL and co-workers in 1944 and by WUL in 1946. The structural change associated with the cubic-tetragonal phase transition was observed, by means of x-rays, by MEGAW in 1945, independently of the above dielectric studies.					42W1, 44O1, 45W1, 44V2, 46W2, 45M1
b	phase	IV <sup>a)</sup>	III <sup>a)</sup>	II <sup>b)</sup>	I <sup>b)</sup>	<sup>a)</sup> 49K2, 49R1
	state	F <sup>a)</sup>	F <sup>a)</sup>	F <sup>c)</sup>	P <sup>b)</sup>	<sup>b)</sup> 45M1
	crystal system	rhombohedral <sup>a)</sup>	orthorhombic <sup>a)</sup>	tetragonal <sup>b)</sup>	cubic <sup>b)</sup>	<sup>c)</sup> 46V1, 46W1
	space group	R3m-C <sub>3v</sub> <sup>a)</sup>	Amm2-C <sub>2v</sub> <sup>a)</sup>	P4mm-C <sub>4v</sub> <sup>b)</sup>	Pm3m-O <sub>h</sub> <sup>b)</sup>	<sup>d)</sup> 55R1
	Θ	-90 <sup>a)</sup>	5 <sup>a)</sup>	120 <sup>b)</sup> **	1460 <sup>d)</sup>	°C
	<p><math>P_s \parallel [001]</math> in phase II (along <math>[100]</math> of phase I).  <math>P_s \parallel [001]</math> in phase III (along <math>[110]</math> of phase I).  <math>P_s \parallel [111]</math> in phase IV (along <math>[111]</math> of phase I).  The directions of <math>P_s</math> are illustrated along with lattice distortions in Fig. 140.  <math>T_{\text{melt}} = 1618^\circ\text{C}</math>.  Tetragonal form (phase II): <math>\rho = 6.02 \cdot 10^3 \text{ kg m}^{-3}</math> (calculated from lattice constants)  <math>a = 3.9920 \text{ \AA}</math>, <math>c = 4.0361 \text{ \AA}</math> at <math>20^\circ\text{C}</math>.  Transparent, light brown.  Hexagonal form: <math>a_{\text{hex}} = 5.735 \text{ \AA}</math>, <math>c_{\text{hex}} = 14.05 \text{ \AA}</math> at RT.  <math>\rho = (6.1 \pm 0.1) \cdot 10^3 \text{ kg m}^{-3}</math>.</p>					51W2, 51R1, 48B3
2a	<p>Crystal growth: Flux method (flux KF<sup>a)</sup> or TiO<sub>2</sub>-rich melt<sup>b)</sup>).  Pulling method (top-seeded solution growth technique using excess TiO<sub>2</sub> as the solvent).  Melting method (with limited success).  Tab. 29; Fig. 141.</p>					<sup>a)</sup> 54R1, <sup>b)</sup> 65S8
b	<p>Crystal forms: For butterfly-type: Fig. 142.  For chunky type: Fig. 143.  For hexagonal form: Fig. 144.</p>					63L3, 50V2
3	<p>Crystal structure of phase I: <math>Z = 1</math>. Tab. 30.  Crystal structure of phase II: <math>Z = 1</math>. Tab. 31.  Crystal structure of phase III: <math>Z = 2</math>. Tab. 32; Fig. 145, 146; Tab. 33.  Crystal structure of phase IV: <math>Z = 1</math>.  Crystal structure of hexagonal form: <math>Z = 6</math>. Tab. 34, 35; Fig. 147.</p>					
4	<p>Lattice constants of phase I, II, III, and IV:  Phase I: <math>a = 3.996 \text{ \AA}</math> at <math>120^\circ\text{C}</math>.  Phase II: <math>a = 3.9920 \text{ \AA}</math>, <math>c = 4.0361 \text{ \AA}</math> at <math>20^\circ\text{C}</math>.  Phase III: <math>a = 3.990 \text{ \AA}</math>, <math>b = 5.669 \text{ \AA}</math>, <math>c = 5.682 \text{ \AA}</math> at <math>-10^\circ\text{C}</math>.  Phase IV: <math>a = 4.001 \text{ \AA}</math>, <math>\alpha = 89^\circ 51'</math> at <math>-168^\circ\text{C}</math>.  Thermal expansion: Fig. 148, 149; Tab. 36, 37; Fig. 150.  Lattice distortion due to <math>p</math>: Fig. 151.</p>					47M3, 51R1, 57S2, 57J2
5a	<p>Dielectric constant: Fig. 152, 153, 154, 192.  Dielectric dispersion: Fig. 155 ... 159.  Further data from optical measurements: Fig. 201; Tab. 42.  Effect of <math>p</math> on <math>\kappa</math>: Fig. 160, 161, 162.  Phase diagram in regard to <math>p</math>: Fig. 163, 164.  Effect of <math>E_{\text{bias}}</math> on <math>\Theta_f</math>: <math>d\Theta_f/dE_{\text{bias}} = 1.43 \cdot 10^{-5} \text{ }^\circ\text{K V}^{-1} \text{ m}</math>; on <math>\kappa</math>: Fig. 165.</p>					53M2
b	<p>Non-linear dielectric properties: Fig. 166.  <math>\xi = -5.5 \cdot 10^8 \text{ J C}^{-4} \text{ m}^5</math>, <math>\zeta = 1.7 \cdot 10^{10} \text{ J C}^{-6} \text{ m}^9</math>.</p>					53M2

\* The transition from the hexagonal form to the cubic one is very sluggish and the hexagonal form can be produced by rapid cooling from above  $1460^\circ\text{C}$ .

\*\* In most papers this Curie point has been reported to be about  $120^\circ\text{C}$ , but it seems to be about  $130^\circ\text{C}$  for pure BaTiO<sub>3</sub> [65J2].



Figure S. 249ff.

## II 1 Oxide des Perowskit-Typs

5c	Nr. 1A-8 BaTiO <sub>3</sub> , continued Spontaneous polarization: Fig. 167, 168, 169. Coercive field: Fig. 170, 171, 172. Effect of $p$ on $P_s$ : Fig. 173.	
d	Electrocaloric effect: Fig. 174. Pyroelectricity: Fig. 175.	
6a	Specific heat: Fig. 176, 177. Transition heat, transition entropy: Tab. 38.	
b	Thermal conductivity: Fig. 178, 179.	
7a	Piezoelectricity: Tab. 39, 40; Fig. 180 ... 183.	
b	Electrostriction: Fig. 184, 185.	
8a	Elastic compliances and stiffnesses: Tab. 41. See also Tab. 40. Fig. 186 ... 193.	
b	Non-linear elastic properties: Fig. 194.	
9a	Refractive indices: Fig. 195, 196, 197. Birefringence: Fig. 198, 199. Reflection and absorption: (i) Far-infrared region. Fig. 200, 201; Tab. 42. (ii) Infrared region. Fig. 202, 203, 204. (iii) Visible region. Fig. 205, 206, 207. (iv) Ultraviolet region. Fig. 208; Tab. 43; Fig. 209, 210, 211. For the effect of $E_{bias}$ on the absorption edge, see	67G1
b	Linear electrooptic effect: Fig. 212 ... 215. Quadratic electrooptic effect: $(M_{11} - M_{12}) = (+ 0.13 \pm 0.02) \text{ m}^4 \text{ C}^{-2}$ at 408 ... 433 °K, measured at 6328 Å.	64G3
d	Faraday rotation: Fig. 216; Tab. 44.	64M2
e	Non-linear optical properties: Susceptibility for SHG (second harmonic generation) (relative values, see Sec. I C): $d_{15} = 35 \pm 3$ , $d_{31} = 37 \pm 3$ , $d_{33} = 14 \pm 1$ , determined with the Nd-doped CaWO <sub>4</sub> laser beam. Fig. 217.	
f	Raman scattering: Fig. 218.	
g	Luminescence: Fig. 219, 220.	
10	Conductivity of as-grown crystals and ceramics: The data vary from sample to sample depending on the purity and the method of preparation: only representative data are given here. Fig. 221 ... 225. Conductivity associated with doping or reduction (including PTC (Positive Temperature Coefficient) or resistivity: $d\rho/dT > 0$ ): Fig. 226 ... 230. Reference papers on PTC anomaly: Tab. 45. Piezoresistivity: Fig. 231, 232. For additional data, see  Breakdown strength: Fig. 233, 234. For additional data, see  Photoconductivity and photoemission: Fig. 235, 236. Other transport properties: In $n$ -type single-domain crystals, the electron mobility is anisotropic at RT; $\mu_{\perp c} \approx 1.2 \cdot 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$ , and $\mu_c \approx 0.13 \cdot 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$ In $n$ -type single-domain crystals, the energy separation ( $\Delta u = 10^{-2} \dots 10^{-1} \text{ eV}$ ) between the $c$ -axis conduction band minima and the $a$ -axis conduction band minima has been estimated vs. $T$ . In $n$ -type single-domain crystals, the density-of-state mass $m^* = (6.5 \pm 2) m_0$ . Data are available on the Hall coefficient and conductivity of single domain crystals having donor concentrations of $N = 8.5 \cdot 10^{24} \text{ m}^{-3}$ and of $N = 2.5 \cdot 10^{23} \text{ m}^{-3}$ . Fig. 237. Seebeck-effect: Fig. 238.	59S1, 63M1, 67G4  58I3, 59F1, 64K3, 64U1  67B2  67B2  67B2 67B2
12b	ESR: Tab. 46; Fig. 239 ... 243.	
c	Mössbauer effect: Fig. 244 ... 247.	
13b	Diffuse X-ray scattering: Fig. 248, 249, 250. Inelastic neutron scattering: Fig. 251.	

14a	Domain structure: Domains have been observed by various methods: polarized light <sup>a)</sup> , X-rays <sup>b)</sup> , electron microscope <sup>c)</sup> , etching method <sup>d)</sup> , powder pattern method <sup>e)</sup> , and decoration method <sup>f)</sup> . Fig. 252 ... 255.	a) 48M1, 49F1, 52M3 b) 63B13, 64N1, 65C3, 64L1 c) 62T1, 63B9, 67R4, 64T2, 66R5, 67R2 d) 55H2 e) 59P1 f) 66S8
b	Domain wall motion: Domain wall motion has been observed optically <sup>a)</sup> and by repeated differential etching <sup>b)</sup> . The domain shapes in motion depend on the applied field and temperature. <sup>c)</sup> Fig. 256.  The wall velocity is proportional to $\exp(-\delta/E)$ at relatively low field. $\delta$ = activation field for domain wall motion. Fig. 257 ... 267.	a) 59M2, 60S2 b) 63S13 c) 63S13  58M4, 59M3
15	Surface layer: The first suggestion about the existence of surface layers of BaTiO <sub>3</sub> crystals was made by KÄNZIG <sup>a)</sup> on the basis of electron diffraction studies of very small particles of BaTiO <sub>3</sub> <sup>b)</sup> . The dependence of the following quantities on the thickness of the crystals has been observed as evidence of the existence of surface layers: domain wall velocity <sup>c)</sup> , dielectric constant <sup>d)</sup> , optical absorption coefficient <sup>e)</sup> and electroluminescence spectra <sup>f)</sup> . Pyroelectric current was observed above the Curie point and discussed in connection with surface layers <sup>g)</sup> . A few models of surface layers have been proposed <sup>h)</sup> . According to TANAKA and HONJŌ <sup>i)</sup> , the surface layer, if it exists, seems to be very thin.	a) 55K1 b) 54A1 c) 56M4, 61M2, 65C1 d) 61S4, 62C3 e) 60C3 f) 58H1, 65B7, 66B6 g) 56C1 h) 56M4, 61F2, 59D3, 65C1 i) 64T2
16	Radiation damage: Fig. 268, 269.	
17	Energy band structure: Fig. 270.	

Tab. 29. BaTiO<sub>3</sub>. Solubility in KF solution. [54K1]

T	1000	1050	1100	1150	1200	1250	1300	°C
BaTiO <sub>3</sub>	4	6	9	12.5	17	22.5	28.5	mole %

Tab. 30. BaTiO<sub>3</sub>. Fractional coordinates of atoms in the unit cell of phase I. [52M2]

	x	y	z
Ba	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
O	$\frac{1}{2}$	$\frac{1}{2}$	0
	$\frac{1}{2}$	0	$\frac{1}{2}$
	0	$\frac{1}{2}$	$\frac{1}{2}$

Tab. 31. BaTiO<sub>3</sub>. Shift of atoms in fractional coordinates of phase II from the positions of phase I. [51K1], [55F1], [61E3]

$\delta z_{Ti}$	$\delta z_{O(1)}$	$\delta z_{O(2)}$	Ba		Ti		O(1)		O(2)			References
			$B_{11}$	$B_{33}$	$B_{11}$	$B_{33}$	$B_{11}$	$B_{22}$	$B_{11}$	$B_{22}$	$B_{33}$	
0.014	-0.032	0	0.48		0.13		0.13		0.48			51K1
0.014	-0.023	-0.014	0.273		0.152		0.334		0.267			55F1
0.015	-0.024	-0.020	0.27	0.28	0.53	0.21	0.90	0.08	0.60	0.49	0.07	61E3
0.012	-0.026	0	0.27	0.28	0.46	0.30	0.90	0.50	0.60	0.90	0.90	61E3

The positions of atoms in the unit cell are Ba at (0, 0, 0), Ti at ( $\frac{1}{2}$ ,  $\frac{1}{2}$ ,  $\frac{1}{2} + \delta z_{Ti}$ ), O(1) at ( $\frac{1}{2}$ ,  $\frac{1}{2}$ ,  $\delta z_{O(1)}$ ) and O(2) at ( $\frac{1}{2}$ , 0,  $\frac{1}{2} + \delta z_{O(2)}$ ).

Tab. 32. BaTiO<sub>3</sub>. Fractional coordinates of atoms in the unit cell of phase III. [57S2]

	<i>x</i>	<i>y</i>	<i>z</i>
Ba	0	0	0
Ti	0	$\frac{1}{2}$	$\frac{1}{2}$
	$\frac{1}{2}$	0	$\frac{1}{2} + \delta z_{Ti}$
	$\frac{1}{2}$	$\frac{1}{2}$	$\delta z_{Ti}$
O(1)	0	0	$\frac{1}{2} + \delta z_{O(1)}$
	0	$\frac{1}{2}$	$\delta z_{O(1)}$
O(2)	$\frac{1}{2}$	$\frac{1}{2} + \delta y_{O(2)}$	$\frac{1}{2} + \delta z_{O(2)}$
	$\frac{1}{2}$	$\frac{3}{4} + \delta y_{O(2)}$	$\frac{3}{4} + \delta z_{O(2)}$
	$\frac{1}{2}$	$\frac{3}{4} - \delta y_{O(2)}$	$\frac{1}{4} + \delta z_{O(2)}$
	$\frac{1}{2}$	$\frac{1}{4} - \delta y_{O(2)}$	$\frac{3}{4} + \delta z_{O(2)}$

$$\delta z_{Ti} = +0.010; \delta z_{O(1)} = -0.010; \delta z_{O(2)} = -0.013;$$

$$\delta y_{O(2)} = +0.003.$$

Tab. 33. BaTiO<sub>3</sub>. Comparison of atomic shifts in phase III and phase II with respect to different origins. The coordinate of atoms of [55F1] and [57S2] are used for phase II and III, respectively. [57S2]

	Orthorhombic	Tetragonal
Ba at (000)		
$\delta z$ { Ti	+0.06 Å	+0.06 Å
O(1)	-0.06 Å	-0.09 Å
O(2)	-0.07 Å	-0.06 Å
$\delta y_{O(2)}$	$\pm 0.02$ Å	-

Origin is chosen to give  $\delta z_{O(2)} = 0$ 

$\delta z$ { Ti	+0.13 Å	+0.15 Å
Ba	+0.07 Å	+0.09 Å
O(1)	+0.02 Å	-0.03 Å

Tab. 34. BaTiO<sub>3</sub>. Fractional coordinates of atoms in the unit cell of hexagonal structure. [48B3]

2Ba(1) at (b),	
4Ba(2) at (f),	$z = 0.097$ ,
2Ti(1) at (a),	
4Ti(2) at (f),	$z = 0.845$ ,
6O(1) at (h),	$x = 0.522$ ,
12O(2) at (k),	$x = 0.836, z = 0.076$

Tab. 35. BaTiO<sub>3</sub>. Interatomic distances of hexagonal structure. [48B3]in the Ti<sub>2</sub>O<sub>7</sub> group

$$O(1) - O(1) = 2.49 \text{ Å}$$

$$= 3.25 \text{ Å}$$

in the shared face.

$$O(2) - O(2) = 2.91 \text{ Å}$$

in the same layer but the atoms do not belong to the same shared face.

$$O(1) - O(2) = 2.91 \text{ Å}$$

$$Ti(2) - O(1) = 1.96 \text{ Å}$$

$$Ti(2) - O(2) = 2.02 \text{ Å}$$

in the TiO<sub>6</sub> octahedra

$$O(2) - O(2) = 2.82 \text{ Å}$$

in the same layer.

$$O(2) - O(2) = 2.69 \text{ Å}$$

$$Ti(1) - O(2) = 1.95 \text{ Å}$$

between adjacent layers.

Tab. 36. BaTiO<sub>3</sub>. Lattice constants and unit cell volume at various *T*. [51R1]

<i>T</i> °C	<i>a</i> Å	<i>b</i> Å	<i>c</i> Å	<i>V</i> Å <sup>3</sup>
+ 20	3.9920	3.9920	4.0361	64.317
+ 4	3.9910	3.9911	4.0357	64.282
Θ <sub>III-II</sub>				
+ 4	4.0185	3.9860	4.0162	64.319
- 99	4.0170	3.9750	4.0150	64.093
Θ <sub>IV-III</sub>				
- 99	4.0015	4.0015	4.0020	64.079
- 160	3.9996	3.9996	3.9997	63.981

Accuracy of measurement below RT was  $\pm 0.0007$  Å.Tab. 37. BaTiO<sub>3</sub>. Linear thermal expansion coefficients along *a*, *b*, and *c* axes. [51R1]

<i>T</i> °C	$\alpha_a$ $10^{-6} \text{ } ^\circ\text{C}^{-1}$	$\alpha_b$ $10^{-6} \text{ } ^\circ\text{C}^{-1}$	$\alpha_c$ $10^{-6} \text{ } ^\circ\text{C}^{-1}$
+20 ... + 4	15.7	15.7	6.2
+ 4 ... - 99	4.9	28.4	-0.9
-99 ... -160	7.8	7.8	8.2

Tab. 38. BaTiO<sub>3</sub>. Transition heats and transition entropies

Transition	$\Delta Q_m$ cal mol <sup>-1</sup>	$\Delta S_m$ cal mol <sup>-1</sup> °K <sup>-1</sup>	References
IV → III	8 ± 2	0.04	52S5
	14.3	0.07	52V1
	12	0.06	52T1
III → II	22 ± 4	0.076	52S5
	15.5	0.054	52V1
	16	0.058	52T1
II → I	50 ± 5	0.125	52S5
	47	0.12	52V1
	47	0.12	48B1

Tab. 39. BaTiO <sub>3</sub> (single crystal and ceramic). Piezoelectric constants and electromechanical coupling factor. [66b1]														
	$d_{15}$	$d_{31}$	$d_{33}$	$10^{-12}$ C N <sup>-1</sup>			$g_{15}$	$g_{31}$	$g_{33}$	$k_p$	$10^8$ C m <sup>-2</sup>			References
				$d_{15}$	$d_{31}$	$d_{33}$					$e_{15}$	$e_{31}$	$e_{33}$	
single crystal	392	57.7 — 34.5 — 33.3 — 103.3	132 85.6 316.6	15.3	— 23.1	57.6	0.570	0.315	0.560					50C2 58B2 59H7 51B1
ceramic	270 260	79 78	191 190	18.8 20.2	4.7 5.2	11.4 12.6	0.476 0.48	0.208 0.212	0.493 0.50	0.378 0.36	11.6 11.4	— 4.4 — 4.35	18.6 17.5	56B3 64b1

  

Tab. 40. BaTiO <sub>3</sub> (ceramic, plain and modified, commercial). Dielectric, piezoelectric, electromechanical and elastic constants (at 25 °C, except for Ca <sub>0.12</sub> Pb <sub>0.08</sub> Ba <sub>0.80</sub> TiO <sub>3</sub> ). [66b1]														
Composition	$\kappa_{33}^T$	$10^{-12}$ C N <sup>-1</sup>			$10^{-3}$ m <sup>2</sup> C <sup>-1</sup>			$k_{15}$	$k_{31}$	$k_{33}$	$k_p$	$10^{-12}$ m <sup>3</sup> N <sup>-1</sup>		
		$d_{15}$	$d_{31}$	$d_{33}$	$g_{15}$	$g_{31}$	$g_{33}$					$s_{11}^E$	$s_{12}^E$	$s_{33}^E$
BaTiO <sub>3</sub>	1350 ...		— 56	130 ...								8.47	— 2.38	21.7
Ca <sub>0.03</sub> Ba <sub>0.97</sub> TiO <sub>3</sub>	1700		— 53	160								8.20	— 2.45	21.3
Ca <sub>0.05</sub> Ba <sub>0.95</sub> TiO <sub>3</sub>	1380		— 58	135								8.6	— 2.6	22.4
Ca <sub>0.08</sub> Ba <sub>0.92</sub> TiO <sub>3</sub> (ceramic B) <sup>a)</sup>	1200	242		149	21.0	— 5.5	14.1	0.48	0.194	0.48	0.33			
Ca <sub>0.09</sub> Ba <sub>0.91</sub> TiO <sub>3</sub>	910		— 41	118								8.00	— 2.40	20.79
Pb <sub>0.04</sub> Ba <sub>0.96</sub> TiO <sub>3</sub>	1000		— 38	105								8.77	— 2.58	22.7
Pb <sub>0.05</sub> Ba <sub>0.95</sub> TiO <sub>3</sub>	1180		— 53	129								9.09	— 2.64	23.64
Ca <sub>0.08</sub> Pb <sub>0.02</sub> Ba <sub>0.90</sub> TiO <sub>3</sub>	800		— 40	115								8.06	— 2.34	20.8
Ca <sub>0.08</sub> Pb <sub>0.02</sub> Ba <sub>0.90</sub> TiO <sub>3</sub>	600		— 29	80								7.63	— 2.87	20.0
Ca <sub>0.08</sub> Pb <sub>0.12</sub> Ba <sub>0.80</sub> TiO <sub>3</sub>	450		— 20	60		— 5.0	15.0	0.30	0.113	0.34	0.19			
Ca <sub>0.12</sub> Pb <sub>0.08</sub> Ba <sub>0.80</sub> TiO <sub>3</sub>	600		— 35	90		— 7.3	18		0.12	0.30	0.22			
	$\kappa_{11}^T$	$\kappa_{11}^S$	$\kappa_{33}^S$	$e_{15}$	$e_{31}$	$e_{33}$	$s_{11}^D$	$s_{33}^D$	$s_{12}^D$	$s_{13}^D$	$s_{33}^D$	$s_{11}^D$	$s_{12}^D$	$s_{33}^D$
				$10^{-12}$ m <sup>3</sup> N <sup>-1</sup>			$10^{-12}$ m <sup>3</sup> N <sup>-1</sup>			$10^{-12}$ m <sup>3</sup> N <sup>-1</sup>			$c_{44}^D$	
Ca <sub>0.08</sub> Ba <sub>0.92</sub> TiO <sub>3</sub> (ceramic B) <sup>a)</sup>	1300	1000	910	10.9	— 3.1	13.5	8.3	9.1	7.0	— 2.9	— 2.7	— 1.9	22.2	17.1
Ca <sub>0.08</sub> Pb <sub>0.12</sub> Ba <sub>0.80</sub> TiO <sub>3</sub>			395				7.7	8.1	7.15	— 2.4				
	$h_{15}$	$h_{31}$	$h_{33}$	$c_{11}^E$	$c_{12}^E$	$c_{33}^E$	$c_{13}^E$	$c_{12}^E$	$c_{13}^E$	$c_{33}^E$	$c_{13}^E$	$c_{44}^E$	$c_{44}^E$	$c_{66}^E$
	$10^8$ N C <sup>-1</sup>			$10^9$ N m <sup>-2</sup>			$10^9$ N m <sup>-2</sup>			$10^9$ N m <sup>-2</sup>			$c_{66}^E$	
Ca <sub>0.08</sub> Ba <sub>0.92</sub> TiO <sub>3</sub> (ceramic B) <sup>a)</sup>	12.3	— 3.8	16.7	158	159	150	177	69	70	67.5	62	45	58.5	45

<sup>a)</sup> Trade Mark: Clevite Corporation, Cleveland, Ohio, USA.

Tab. 41. BaTiO<sub>3</sub> (single crystal and ceramics). Elastic constants. [66bf]

	$10^{-12} \text{ m}^2 \text{ N}^{-1}$										$T$ °C	References
	$s_{11}^E$	$s_{11}^D$	$s_{11}^E$	$s_{11}^D$	$s_{12}^E$	$s_{12}^D$	$s_{13}^E$	$s_{13}^D$	$s_{44}^E$	$s_{44}^D$		
single crystal	9.26 11.2 8.05	7.25	15.7	10.8	-2.35	-3.15	-5.24	-3.26	18.4	12.4	25 RT 25	50C2 51B1 58B2
ceramics	8.55 9.1	8.18 8.7	8.93 9.5	6.76 7.1	-2.61 -2.7	-2.98 -3.0	-2.85 -2.9	-1.95 -1.9	23.3 22.8	18.3 17.5	25 25	56B3 64b1
	$c_{11}^E$	$c_{11}^D$	$c_{33}^E$	$c_{33}^D$	$c_{12}^E$	$c_{12}^D$	$c_{13}^E$	$c_{13}^D$	$c_{44}^E$	$c_{44}^D$		
single crystal	275.1	282.6 206	164.9	178.1	179.0	186.5 140	151.6	141.6	54.34	80.64 126	25 RT	66b1, 58B2 51B1
ceramics	166 150 165.6	168 150	162 146	189 171 180.7	76.6 66	78.2 68	77.5 66	71.0 57	42.9 44	54.6 57	25 25 25	56B3 64b1 55H5

Tab. 42 ... 45 see page 58

Tab. 46. BaTiO<sub>3</sub>. Summary of the ESR parameters for various paramagnetic centers in doped BaTiO<sub>3</sub>.

Para-magnetic center	Site	S	g	$\nu$ GHz	T °K	g-factor	FS		HFS		Ref.	Literature
							$D, E, a, F [10^{-2} \text{ m}^{-1}]$		I	$A, B [10^{-2} \text{ m}^{-1}]$		
Mn <sup>2+</sup>	Ti <sup>4+</sup>	5/2	(7)	9.3	78	2.0016 ± 0.0005	$D = 56 \pm 5$		5/2	$^{55}\text{A}_{  } = ^{55}\text{A}_{\perp} = 79.8 \pm 0.5$	a)	60I1
					300	2.0023 ± 0.0005	$D = 65 \pm 5$			$^{55}\text{A}_{  } = 78.6 \pm 0.5$	b)	63O1
					440	2.0009 ± 0.001	$a = 14 \pm 5$			$^{55}\text{A}_{  } = 79 \pm 0.5$	c)	64I5
	Ba <sup>2+</sup>	5/2	(7)	9.3	RT	2.002 ± 0.001	$D = +(215 \pm 2)$ $a = +(16.76 \pm 0.94)$			$^{55}\text{A}_{  } = -(77.4 \pm 0.6)$ $^{55}\text{A}_{\perp} = -(82.3 \pm 0.8)$		
					438	2.002 ± 0.001	$D = 0$ $a = +(12.11 \pm 0.94)$			$^{55}\text{A}_{  } = ^{55}\text{A}_{\perp} = -(79.3 \pm 0.4)$		66I31)2)

Para-magnetic center	Site	S	g	$\nu$ GHz	T °K	g-factor	FS		HFS		Ref.	Literature
							$D, E, a, F, b [10^{-2} \text{ m}^{-1}]$		I	$A, B [10^{-2} \text{ m}^{-1}]$		

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Tab. 42. BaTiO<sub>3</sub>, SrTiO<sub>3</sub>, TiO<sub>2</sub>, KTaO<sub>3</sub>. Dispersion parameters calculated from the Kramers-Kronig analysis [62S11]. See Fig. 201
$$\kappa' = \kappa_{\infty} + \sum_i 4\pi\epsilon_i \nu_i^2 \frac{\nu_i^2 - \nu^2}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2} \quad \kappa'' = \sum_i 4\pi\epsilon_i \nu_i^2 \frac{\gamma_i \nu}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2}$$

	BaTiO <sub>3</sub> Ordinary ray	SrTiO <sub>3</sub>	TiO <sub>2</sub> Ordinary ray	KTaO <sub>3</sub>
$\lambda_1; \nu_1$	20.4; 491	18.4; 544	20.0; 500	18.2 ± 0.2; 549 ± 6
$\gamma_1/\nu_1$	0.059 ± 0.002	0.049 ± 0.002	0.044 ± 0.004	0.043 ± 0.009
$4\pi\epsilon_1$	0.60 ± 0.03	1.56 ± 0.06	2.0 ± 0.2	2.4 ± 0.5
$\lambda_2; \nu_2$	54.8; 183	56.3 ± 0.5; 178 ± 2.0	25.8; 388	49.8; 200.8
$\gamma_2/\nu_2$	0.030 ± 0.006	0.039 ± 0.004	0.058 ± 0.006	0.055 ± 0.011
$4\pi\epsilon_2$	2.2 ± 0.4	3.6 ± 0.4	1.08 ± 0.1	7.6 ± 1.5
$\lambda_3; \nu_3$	296 ± 8; 33.8 ± 0.9	114.3 ± 1.1; 87.7 ± 0.9	54.8 ± 0.5; 183 ± 1.8	107.5 ± 2.0; 93.0 ± 2.0
$\gamma_3/\nu_3$	2.5 ± 0.1	0.5 ± 0.1	0.19 ± 0.01	0.5 ± 0.1
$4\pi\epsilon_3$	1830 ± 70	311 ± 62	81.5 ± 4.1	163 ± 33

Resonance wavelength  $\lambda_i$  in 10<sup>-6</sup> m; resonance frequency  $\nu_i$  in 10<sup>2</sup> m<sup>-1</sup>; width  $\gamma_i$ ; strength  $4\pi\epsilon_i$ .Tab. 43. BaTiO<sub>3</sub>, SrTiO<sub>3</sub>, TiO<sub>2</sub>. Energies of fundamental absorption edges (in eV) at RT. [65C2]

	$E_0$	$A_1$	$A_2$	$A_3$	$B_1$	$B_2$	$C_1$	$C_2$	$D$	$E$	
SrTiO <sub>3</sub>	3.2	4.00	4.86	5.5	6.52	7.4	9.2	9.9	12.5	15.3	eV
BaTiO <sub>3</sub>	3.2	3.91	4.85		6.10	7.25	10.3	11.8	12.8	15	eV
TiO <sub>2</sub> ( $E \perp c$ )		3.97	5.52		6.50	7.64	8.53	9.24	11	14.1	eV

Tab. 44. BaTiO<sub>3</sub>, SrTiO<sub>3</sub>, KTaO<sub>3</sub>, KTa<sub>0.35</sub>Nb<sub>0.65</sub>O<sub>3</sub> (KTN), TiO<sub>2</sub>. Band gap energies  $\hbar\omega_g$  (in eV). [67B1]. See Fig. 46, 103, 216, 430.  $F_1, F_2$ : different dispersion functions  $F_i(\omega/\omega_g)$ , see [67B1]

	SrTiO <sub>3</sub>		BaTiO <sub>3</sub>	KTaO <sub>3</sub>		KTN	TiO <sub>2</sub>	
	296 °K	77 °K	403 °K	296 °K	77 °K	296 °K	296 °K	
Faraday rotation $\hbar\omega_g$ for $F_1$	3.40	3.43	3.25	3.77	3.79	3.54	3.62	eV
Faraday rotation $\hbar\omega_g$ for $F_2$	3.21	3.26	3.11	3.62	3.65	3.36	3.37	eV
Energy of reflectivity peak or shoulder	3.20	—	3.20	—	—	3.70	—	eV
Energy of electroreflectance singularity	—	—	3.20	3.57	—	3.60	3.00	eV
$\hbar\omega_g$ from absorption data	3.40	—	—	3.80	—	—	3.30	eV
Energy at which absorption coefficient $\alpha \approx 10^4$ cm <sup>-1</sup>	3.37	—	3.26	3.79	—	3.45	3.18	eV

Tab. 45. BaTiO<sub>3</sub> (reduced or doped). List of reference papers on PTC anomaly

Materials (dopants)	References	Materials (dopants)	References
Single crystal BaTiO <sub>3</sub> : reduced	57H1, 63K3, 64I4, 64G4, 65M1, 65U2	Ceramics BaTiO <sub>3</sub> : La	63H5, 65U2, 59S1, 63T3, 64J1, 65M1
BaTiO <sub>3</sub> : Nb	64B11	BaTiO <sub>3</sub> : Ce	63T3
		BaTiO <sub>3</sub> : Sm	63G5
		BaTiO <sub>3</sub> : Gd	65U2
		BaTiO <sub>3</sub> : Sb	65A3
		(Ba-Sr)TiO <sub>3</sub>	61H5, 65A3
		(Ba-Sr)TiO <sub>3</sub> : La	59S1, 61T1, 63T3
		BaTiO <sub>3</sub> : Sr, Ce, Sn	61S1
		BaTiO <sub>3</sub> : Sr, Ca, Sn	61S1
		BaTiO <sub>3</sub> : Sr, Bi	63T3
		BaTiO <sub>3</sub> : Mg, Ce	61S1
		BaTiO <sub>3</sub> : Zr, Ce	61S1
		BaTiO <sub>3</sub> : Si, Ce	61S1

Nr. 1A-9 PbTiO<sub>3</sub>, Lead titanate

1a	Ferroelectric activity was reported independently by SHIRANE et al. and by SMOLENSKII in 1950.			50S4 50S6	
b	phase	III <sup>b</sup> )*	II <sup>a</sup> )	I <sup>a</sup> )	
	state		F <sup>a</sup> )	P <sup>a</sup> )	
	crystal system		tetragonal <sup>c</sup> )	cubic <sup>a</sup> )	
	space group		P4mm-C <sub>4v</sub> <sup>1</sup>	Pm3m-O <sub>h</sub> <sup>1</sup>	
	Θ	-100 <sup>b</sup> )      490 <sup>a</sup> )      °C			
a = 3.904 <sub>5</sub> Å, c = 4.152 <sub>4</sub> Å at RT (in phase II).					46M2
2a	Crystal growth: KF flux method; PbCl <sub>2</sub> flux method.				58K1, 52N2
b	Crystal form: Fig. 271.				
3	Crystal structure: Positional parameters: Tab. 47, 48. Projection of crystal structure: Fig. 272, 273.				
4	Thermal expansion: Fig. 274 ... 280. Dependence of lattice parameters on hydrostatic pressure: Fig. 281.				
5a	Dielectric constants: Fig. 282. Small dielectric anomaly was observed at about -100 and -150 °C. Curie-Weiss constant: C = 1.1 · 10 <sup>5</sup> °K (single crystal).				56K2 62B4
6a	Specific heat: Fig. 283.				
		II-I			
	ΔQ <sub>m</sub>	1150	cal mol <sup>-1</sup>		51S7
	ΔS <sub>m</sub>	1.6	cal °K <sup>-1</sup> mol <sup>-1</sup>		51S7
c	Thermal conductivity: Fig. 284.				
7a	Piezoelectric properties: Tab. 49.				
9a	Birefringence: Fig. 285. Infrared absorption: Fig. 286, 287. Frequencies of infrared modes: Tab. 50.				
12b	ESR: Tab. 51.				
14a	Domain structures were observed by polarized light.				52N2, 58K1, 59K1
16	Radiation damage: Fig. 288.				

Tab. 47. PbTiO<sub>3</sub>. Positional parameters of atoms at RT. [56S5]

	x	y	z
Pb	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	0.540
O(1)	$\frac{1}{2}$	$\frac{1}{2}$	0.112
O(2)	$\frac{1}{2}$	0	0.612
	0	$\frac{1}{2}$	0.612

Tab. 48. PbTiO<sub>3</sub>. Bond lengths in Å at RT (phase II) and at 490 °C (phase I) [56S5]. O(1)<sub>+</sub> represents the O(1) ion closer to, O(1)<sub>-</sub> that further away from Ti. Similarly O(2)<sub>+</sub> is closer to Pb

phase	II (at RT)	I (at 490 °C)
Ti-O(1) <sub>+</sub>	1.78	1.89
Ti-O(1) <sub>-</sub>	2.38	
Ti-O(2)	1.98	
Pb-O(1)	2.80	2.80
Pb-O(2) <sub>+</sub>	2.53	
Pb-O(2) <sub>-</sub>	3.20	

\* Phase transition II-III was reported to occur only if the cooling rate is extremely slow. [55K3]



Tab. 49.  $\text{PbTiO}_3$  (modified ceramics). Electromechanical constants at RT. [68U1]

Additive	$\text{PbNb}_{4/5}\text{O}_3$ 5.0 mol%	$\text{BiZn}_{1/2}\text{Ti}_{1/2}\text{O}_3$ 5.0 mol%	$\text{Bi}_{2/3}\text{Zn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ 5.0 mol%	
$a$	3.915	3.904	3.911	Å
$c$	4.104	4.148	4.133	Å
$c/a$	1.049	1.062	1.057	
$\rho$	7.19	7.68	7.12	$10^3 \text{ kg m}^{-3}$
porosity	0.105	0.036	0.10	
$\Theta$	466	524	494	$^\circ\text{C}$
$\kappa_{11}^T$	—	195	244	
$\kappa_{33}^T$	226	147	203	
$d_{31}$	10	3.9	7.4	$10^{-12} \text{ C N}^{-1}$
$d_{33}$	37	37	47	$10^{-12} \text{ C N}^{-1}$
$g_{31}$	5.2	3.0	4.1	$10^{-3} \text{ m}^2 \text{ C}^{-1}$
$g_{33}$	16	28	28	$10^{-3} \text{ m}^2 \text{ C}^{-1}$
$s_{11}^E$	1.2	1.2	1.1	$10^{-11} \text{ m}^2 \text{ N}^{-1}$
$s_{33}^E$	1.1	0.95	1.1	$10^{-11} \text{ m}^2 \text{ N}^{-1}$
$Q_{\text{mech}}$ for $s_{11}$	336	54	326	
for $s_{33}$	71	74	76	
$k_{15}$	—	0.40	0.36	
$k_{31}$	0.068	0.031	0.052	
$k_{33}$	0.23	0.32	0.35	

Tab. 50.  $\text{PbTiO}_3$ . Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Ti-O stretch)	$\tilde{\nu}_2$ (Ti-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Ti-O bend)	$\tilde{\nu}_4$ (cation-TiO <sub>3</sub> lattice mode)
530 ( $E_u, A_1$ )	400 ( $B_1, E_u$ )	220 ( $E_u, A_1$ ) 172	83 ( $E_u, A_1$ )

Tab. 51.  $\text{PbTiO}_3$ .  $g$ -factors at RT. [64G1]

Paramagnetic center	Site	$S$	$\mathcal{H}$	$\nu$ GHz	$T$ $^\circ\text{K}$	$g$ -factor	
						$g_{\parallel}$	$g_{\perp}$
$\text{Fe}^{3+}$	$\text{Ti}^{4+}$	$1/2^*$	(2)	8.8	RT	$2.009 \pm 0.005$	$5.97 \pm 0.02$

The spectrum up to 300  $^\circ\text{C}$  and down to  $-120$   $^\circ\text{C}$  did not show any fundamental change.

Nr. 1A-10  $\text{CaZrO}_3$ , Calcium zirconate

1	A few physical properties of $\text{CaZrO}_3$ were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be orthorhombic with the cell dimensions $a = 5.587$ Å, $b = 8.008$ Å, $c = 5.758$ Å at RT.	
4	Linear thermal expansion: $\alpha = 8.55 \cdot 10^{-6} \text{ }^\circ\text{C}^{-1}$ between 23 $^\circ\text{C}$ and 223 $^\circ\text{C}$ ; $\alpha = 9.53 \cdot 10^{-6} \text{ }^\circ\text{C}^{-1}$ between 223 $^\circ\text{C}$ and 333 $^\circ\text{C}$ for ceramics of bulk density $\rho = 4.95 \cdot 10^3 \text{ kg m}^{-3}$	55C1 65B10
9	Infrared absorption: Fig. 289, 290; Tab. 52.	

Tab. 52.  $\text{CaZrO}_3$ . Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
515 ( $B_1, B_2, A_1$ )	340 ( $B_1, B_2, A_2$ ) (377) (418)	228 ( $B_1, B_2, A_1$ ) 186	153 ( $B_1, B_2, A_1$ ) 96

\* The fictitious spin is  $\frac{1}{2}$  [64G1].

Nr. 1A-11 SrZrO<sub>3</sub>, Strontium zirconate

1	A few physical properties of SrZrO <sub>3</sub> were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be pseudo-cubic with $a' = 4.099 \text{ \AA}$ at RT.	57R2
4	Linear thermal expansion: $\alpha = 8.75 \cdot 10^{-6} \text{ }^\circ\text{C}^{-1}$ between 23 °C and 320 °C; $\alpha = 9.34 \cdot 10^{-6} \text{ }^\circ\text{C}^{-1}$ between 320 °C and 700 °C for ceramics of bulk density $\rho = 5.00 \cdot 10^3 \text{ kg m}^{-3}$ .	65B10
9	Infrared absorption: Fig. 291, 292; Tab. 53.	

Tab. 53. SrZrO<sub>3</sub>. Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
522 ( $B_1, B_2, A_1$ )	325 ( $B_1, B_2, A_2$ ) (357) (379)	240 ( $B_1, B_2, A_1$ )	143 ( $B_1, B_2, A_1$ )

Nr. 1A-12 BaZrO<sub>3</sub>, Barium zirconate

1	A few properties of BaZrO <sub>3</sub> were reported in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be cubic with the cell dimensions $a = 4.192 \text{ \AA}$ at RT.	57R2
4	Linear thermal expansion: $\alpha = 5.64 \cdot 10^{-6} \text{ }^\circ\text{C}^{-1}$ between 23 °C and 214 °C; $\alpha = 6.54 \cdot 10^{-6} \text{ }^\circ\text{C}^{-1}$ between 214 °C and 324 °C for ceramics of bulk density $\rho = 6.73 \cdot 10^3 \text{ kg m}^{-3}$ .	65B10
9	Infrared absorption: Fig. 293, 294; Tab. 54.	

Tab. 54. BaZrO<sub>3</sub>. Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
505 ( $F_{1u}$ )	— ( $F_{2u}$ )	210 ( $F_{1u}$ )	115 ( $F_{1u}$ )

Nr. 1A-13 PbZrO<sub>3</sub>, Lead zirconate

1a	Dielectric anomaly of PbZrO <sub>3</sub> associated with a phase transition was reported independently by ROBERT and by SMOLENSKII in 1950. Antiparallel ionic shifts on the (001) projection of crystal structure were found by SAWAGUCHI et al. in 1951. In the same year antiferroelectric double hysteresis loops were discovered by SHIRANE et al.. PbZrO <sub>3</sub> is the first compound in which double hysteresis loops were observed.		50R1, 50S7 51S3 51S8
b.	phase	II <sup>a</sup> )	I <sup>a</sup> )
	state	A <sup>b</sup> )	P <sup>a</sup> )
	crystal system	orthorhombic <sup>c</sup> )	cubic <sup>c</sup> )
	space group	Pba2-C <sub>2v</sub> <sup>c</sup> )	Pm3m-O <sub>h</sub> <sup>c</sup> )
	230 °C <sup>a</sup> )		51S3
	$\Theta$ $a = 5.87 \text{ \AA}$ , $b = 11.74 \text{ \AA}$ , $c = 8.20 \text{ \AA}$ at RT (in phase II): The cubic unit cell in phase I becomes pseudo-tetragonal in phase II. The pseudo-tetragonal cell constants $a'$ and $c'$ are related with the orthorhombic cell constants $a$ , $b$ and $c$ : $a = \sqrt{2} a'$ , $b = 2\sqrt{2} a'$ and $c = 2c'$ , where $a' = 4.15 \text{ \AA}$ , $c' = 4.10 \text{ \AA}$ at RT. Relation between the pseudo-tetragonal and orthorhombic cells: Fig. 295.		55J2
2a	Crystal growth: PbCl <sub>2</sub> flux method.		

3	Nr. 1A-13 PbZrO <sub>3</sub> continued Z = 8 (in phase II). The crystal is polar along the <i>c</i> axis and antipolar along the <i>a</i> axis in phase II. Fig. 295 shows schematically the shifts of Pb ions. Positional parameters and shifts from ideal perovskite positions: Tab. 55. Projection of ZrO <sub>6</sub> : Fig. 296, 297, 298. Bond distances between Zr and O: Fig. 299.	51S3, 57J4, 51S3 57J4
4	Thermal expansion: Fig. 300 ... 303. $\alpha_a \cong -0.05 \cdot 10^{-5} \text{ }^\circ\text{K}^{-1}$ and $\alpha_c \cong 2.80 \cdot 10^{-5} \text{ }^\circ\text{K}^{-1}$ in phase II; $\alpha_a \cong 1.10 \cdot 10^{-5} \text{ }^\circ\text{K}^{-1}$ in phase I, where $\alpha_a$ and $\alpha_c$ are the linear thermal expansion coefficients along the pseudo-tetragonal <i>a'</i> and <i>c'</i> axes, respectively.	52S1
5a	Dielectric constants: Fig. 304. $C = 1.36 \cdot 10^5 \text{ }^\circ\text{K}$ (determined with ceramics). Effect of pressure: Fig. 305. $(d\epsilon_a/dp)_{p \rightarrow 0} = (4.1 \pm 0.2) 10^{-8} \text{ }^\circ\text{K N}^{-1} \text{ m}^2$ .	50R1 66R2
c	Critical field: Fig. 306.	
6a	Specific heat: Fig. 307. For the transition II-I: $\Delta Q_m = 440 \text{ cal mol}^{-1}$ ; $\Delta S_m = 0.88 \text{ cal }^\circ\text{K}^{-1} \text{ mol}^{-1}$ .	
b	Thermal conductivity: Fig. 308.	52S2
8	Elastic compliances: Fig. 309.	
9a	Birefringence: Fig. 310. Infrared absorption: Fig. 311, 312; Tab. 56.	
16	Radiation damage: Fig. 313.	

Tab. 55. PbZrO<sub>3</sub> (ceramics). Atomic coordinates and shifts from ideal perovskite positions at RT. [57J4]

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Wyckoff notation	Total shift Å
Pb'	0.706	0.127	0	4 <i>c</i>	0.26
Pb''	0.706	0.127	0.500	4 <i>c</i>	0.26
Zr'	0.243	0.124	0.250	4 <i>c</i>	0.04
Zr''	0.243	0.124	0.250	4 <i>c</i>	0.04
O(1)'	0.270	0.150	0.980	4 <i>c</i>	0.35
O(1)''	0.270	0.100	0.480	4 <i>c</i>	0.35
O(2)'	0.040	0.270	0.300	4 <i>c</i>	0.53
O(2)''	0.040	0.270	0.750	4 <i>c</i>	0.34
O(3)'	0	0.500	0.250	2 <i>b</i>	0
O(3)''	0	0.500	0.800	2 <i>b</i>	0.41
O(4)'	0	0	0.250	2 <i>a</i>	0
O(4)''	0	0	0.800	2 <i>a</i>	0.41

Tab. 56. PbZrO<sub>3</sub>. Wave numbers in  $10^3 \text{ m}^{-1}$  and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
508 ( <i>E<sub>u</sub></i> , <i>A<sub>1</sub></i> )	290 ( <i>B<sub>1</sub></i> , <i>E<sub>u</sub></i> )	221 ( <i>E<sub>u</sub></i> , <i>A<sub>1</sub></i> )	80 ( <i>E<sub>u</sub></i> , <i>A<sub>1</sub></i> ) 34

Nr. 1A-14 PbHfO<sub>3</sub>, Lead hafnate

1a	A dielectric anomaly associated with a phase transition was observed, and the possibility of the antiferroelectricity was discussed by SHIRANE et al. in 1953.				53S3
b	phase	III	II	I	53S3
	state	(A)		P	
	crystal system	pseudo-tetragonal	tetragonal	cubic	
	Θ	163	215	°C	
	Lattice constants for the pseudo-tetragonal phase: <i>a'</i> = 4.136 Å, <i>c'</i> / <i>a'</i> = 0.991 at RT.				53S3

4	Thermal expansion: Fig. 314. Cubic thermal expansion coefficients: below 158 °C: $20 \cdot 10^{-6} \text{ deg}^{-1}$ ; above 215 °C: $27 \cdot 10^{-6} \text{ deg}^{-1}$ .	53S3																									
5a	Dielectric constant: Fig. 315. $C = 9.5 \cdot 10^4 \text{ }^\circ\text{K}$ (ceramics).	53S3																									
Nr. 1A-15 BiFeO <sub>3</sub> , Bismuth ferrite																											
1a	In 1960 <sup>a</sup> ) it was pointed out on the basis of x-ray studies of the solid solution, PbTiO <sub>3</sub> -BiFeO <sub>3</sub> , that BiFeO <sub>3</sub> could have a ferroelectric Curie point at high temperatures. The Curie point was estimated to be about 850 °C from studies of the same solid solution <sup>b</sup> ). Disagreement, however, exists among many experimental data reported so far, therefore reservation is necessary in deciding whether BiFeO <sub>3</sub> is ferroelectric or antiferroelectric. Antiferromagnetic anomaly in BiFeO <sub>3</sub> was observed by direct magnetic measurements at about 370 °C <sup>c</sup> ).	<sup>a</sup> )60F9, 60V2  <sup>b</sup> )61F3, 62F8  <sup>c</sup> )62S10, 63R1, 65I2																									
b	<table><tr><td>phase</td><td>IV</td><td>III</td><td>II</td><td>I</td></tr><tr><td>state</td><td>(A) or (F), <math>A_{\text{magn}}^*</math></td><td>(A) or (F), <math>P_{\text{magn}}</math></td><td>(A) or (F), <math>P_{\text{magn}}</math></td><td>(P), <math>P_{\text{magn}}</math></td></tr><tr><td>crystal system</td><td>rhombohedral</td><td>rhombohedral</td><td>rhombohedral</td><td>cubic (possibly)</td></tr><tr><td>space group</td><td>R3m-C<sub>3v</sub><sup>**</sup></td><td></td><td></td><td></td></tr><tr><td><math>\theta</math></td><td colspan="4">370                      <math>\approx</math>575                      850                      °C</td></tr></table> <p><math>a = (3.962 \pm 0.001) \text{ \AA}</math>, <math>\alpha = 89^\circ 31' \pm 3'</math> at RT. Further references are available on unit cell parameters.</p>	phase	IV	III	II	I	state	(A) or (F), $A_{\text{magn}}^*$	(A) or (F), $P_{\text{magn}}$	(A) or (F), $P_{\text{magn}}$	(P), $P_{\text{magn}}$	crystal system	rhombohedral	rhombohedral	rhombohedral	cubic (possibly)	space group	R3m-C <sub>3v</sub> <sup>**</sup>				$\theta$	370 $\approx$ 575                      850                      °C				64T6 60V2, 60F6, 60Z2
phase	IV	III	II	I																							
state	(A) or (F), $A_{\text{magn}}^*$	(A) or (F), $P_{\text{magn}}$	(A) or (F), $P_{\text{magn}}$	(P), $P_{\text{magn}}$																							
crystal system	rhombohedral	rhombohedral	rhombohedral	cubic (possibly)																							
space group	R3m-C <sub>3v</sub> <sup>**</sup>																										
$\theta$	370 $\approx$ 575                      850                      °C																										
3	Crystal structure: From the x-ray diffraction studies, BiFeO <sub>3</sub> was found to belong to one of the five space groups: R 3, $R \bar{3}$ , R 32, R3m and $R\bar{3}m$ . Neutron diffraction studies suggested that BiFeO <sub>3</sub> belongs to the non-centrosymmetric space group R3m. The crystal structure can be regarded as consisting of alternating FeO <sub>6</sub> and BiO <sub>6</sub> trigonal pyramids: Fig. 316; Tab. 57. According to the electron diffraction study, BiFeO <sub>3</sub> belongs to the non-centrosymmetric space group R3m at RT. Atomic coordinates: Tab. 58. The space group $R\bar{3}m$ was, however, rejected by SMOLENSKII et al., because it does not satisfy the conditions for the existence of weak ferromagnetism. The magnetic structure of BiFeO <sub>3</sub> was proved to be G-type by the neutron diffraction experiments. Fig. 317, 318.	60Z2 63K5  64T6  64S9 63K5																									
4	Unit cell parameters: Fig. 319, 320. See also	66R8, 64T5																									
5a	Dielectric constant: Fig. 321, 322, 323. No reliable data on the dielectric constant in the high temperature region near 850 °C are available.																										
11	Magnetic susceptibility: Fig. 324. At RT, no spontaneous magnetic moment was observed in the fields up to 22 kOe.																										
12c	Mössbauer effect: Fig. 325, 326.																										
17	Calculations of the internal electric fields and their gradients in BiFeO <sub>3</sub> crystals were made on the basis of an ionic model.	67T7																									
Tab. 57. BiFeO <sub>3</sub> . Values of the interatomic distances [Å]. [63K5]. See Fig. 316. See also [64T6]																											
	520 °C	20 °C																									
Bi-Fe (A)	3.841	3.857																									
Bi-Fe (B)	3.006	2.994																									
Bi-O (C)	2.903	2.907																									
Bi-O (D)	2.680	2.693																									
Fe-O (F)	2.233	2.214																									
Fe-O (G)	1.754	1.774																									
O-O (H)	2.841	2.859																									
O-O (K)	2.800	2.800																									
O-O (L)	2.680	2.724																									
Tab. 58. BiFeO <sub>3</sub> . Atomic coordinates. [64T6]																											
Atom	x	y	z																								
Bi	0.0337	0.0337	0.0337																								
Fe	0.5000	0.5000	0.5000																								
O(1)	-0.0280	0.5000	0.5000																								
O(2)	0.5000	-0.0280	0.5000																								
O(3)	0.5000	0.5000	-0.0280																								
* This state is presumably weak ferromagnetic. [66Y2] ** See subsection 3.																											

Classification of Perovskite-Typ

Nr. 1A-16 KIO<sub>3</sub>, Potassium iodate

1a	Ferroelectric behavior in KIO <sub>3</sub> was reported by HERLACH in 1961.						61H3
b	phase	V <sup>a)</sup>	IV <sup>a)</sup>	III <sup>a)</sup>	II <sup>a)</sup>	I <sup>a)</sup>	<sup>a)</sup> 61H3
	state		F <sup>a)</sup>	F <sup>a)</sup>	F <sup>a)</sup>	P <sup>a)</sup>	
	crystal system			trigonal <sup>b)</sup> *		trigonal <sup>a)</sup>	<sup>b)</sup> 60S5
	Θ	−190 <sup>a)</sup>	−18, −10 <sup>a)</sup> **	70 <sup>a)</sup>	212 <sup>a)</sup>	°C	
	$T_{\text{melt}} = 560\text{ }^{\circ}\text{C}$ . $\rho = 3.979^{1)} \cdot 10^3\text{ kg m}^{-3}$ . <sup>1)</sup> A different value, 3.802, is also given in the same reference. $a = (4.410 \pm 0.005)\text{ \AA}$ , $\alpha = 89,41^{\circ}$ at RT, adopting trigonal system. $a = 8.921\text{ \AA}$ , $b = 8.916\text{ \AA}$ , $c = 8.885\text{ \AA}$ , $\alpha \cong \beta \cong \gamma \cong 90^{\circ} \pm 30'$ at RT, adopting triclinic system. Transparent						66H17 08g1 60S5 65F3
2a	Hydrothermal method: Fig. 327. Growth from the supersaturated solution with 10 ... 14% HIO <sub>3</sub> at a constant temperature: Fig. 328.						61H3 27m1
3	$Z = 1$ in phase III, adopting trigonal system. $Z = 8$ in phase III, adopting triclinic system.						61H3 65F3
4	Lattice deformation: $a = [4.44 + 0.00022 (T - 220)]\text{ \AA}$ , $\alpha = 89^{\circ} 20' - 0.09 (T - 220)'$ in phase I ( $T$ in $^{\circ}\text{C}$ ).						61H3
5a	Dielectric constants: Fig. 329, 330.						66H17
c	Spontaneous polarization: Fig. 331.						61H3
9a	Absorption edge: Fig. 332.						67V2
12a	NMR: Fig. 333.						61H3

1B Complex perovskite-type oxides

Nr. 1B1-i (K<sub>1/2</sub>Bi<sub>1/2</sub>)TiO<sub>3</sub>, Potassium bismuth titanate

1a	Ferroelectricity in (K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> was found by SMOLENSKII and AGRANOVSKAYA in 1959.						59S6
b	phase	III	II	I			
	state	(F)	(A)	P			
	crystal system	tetragonal	pseudo-cubic	cubic			62I5
	space group			Pm3m-O <sub>h</sub>			
	Θ	270	410,380 <sup>a)</sup>	°C			<sup>a)</sup> 60S6
	$a = (3.913 \pm 0.003)\text{ \AA}$ , $c = (3.993 \pm 0.003)\text{ \AA}$ at RT.						
3	Crystal structure: Disordered perovskite.						62I5
4	Lattice distortion: Fig. 334. Thermal expansion: Fig. 335.						
5a	Dielectric constant: Fig. 336.						

Nr. 1B1-ii (Na<sub>1/2</sub>Bi<sub>1/2</sub>)TiO<sub>3</sub>, Sodium bismuth titanate

1a	Ferroelectricity in (Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> was found by SMOLENSKII and AGRANOVSKAYA in 1959.						59S6
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\* Various crystal systems have been proposed: trigonal [60S5], triclinic [65F3].  
 \*\* −10  $^{\circ}\text{C}$  on heating, −18  $^{\circ}\text{C}$  on cooling.

\* Various crystal systems have been proposed: trigonal [60S5], triclinic [65F3].  
 \*\* -10  $^\circ\text{C}$  on heating, -18  $^\circ\text{C}$  on cooling.

1b	
3	
4	
5a	
c	
Nr.	
1a	
b	
2a	
3	
4	
5a	
6	
8a	
Nr. 1	
1a	
b	
3	
4	
5a	

1b	phase	III	II	I	62I5
	state	F	(A)	P	
	crystal system	rhombohedral	pseudo-cubic	cubic	
	space group			Pm3m-O <sub>h</sub> <sup>1</sup>	
	Θ	≈200 <sup>a</sup> ) 320 °C			
a = (3.891 ± 0.002) Å, α = 89° 36' ± 3' at RT.					
3	Crystal structure: Disordered perovskite.				62I5
4	Thermal expansion: Fig. 337.				
5a	Dielectric constant: Fig. 338.				60S6
c	Spontaneous polarization and coercive field: P <sub>s</sub> ≈ 8.0 · 10 <sup>-2</sup> C m <sup>-2</sup> ; E <sub>c</sub> ≈ 14 · 10 <sup>2</sup> kV m <sup>-1</sup> at 116 °C.				
Nr. 1B2-i Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>					
1a	Antiferroelectric properties of Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> were discovered by SMOLENSKII et al. in 1959.				59S7
b	phase	II	I		62Z1
	state	A	P		
	crystal system	orthorhombic	cubic		
	space group	C222 <sub>1</sub> -D <sub>2</sub> <sup>2</sup>			
	Θ	38 °C			
a = 22.74 Å, b = 22.79 Å, c = 15.90 Å at RT. Orthorhombic unit cell: see Fig. 339.					
2a	Crystal growth: Crystal growth of Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> was reported by MYL'NIKOVA.				60M2
3	Crystal structure: Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> has the structure of perovskite type. Fig. 339. Z = 64 (molecular unit: Pb <sub>2</sub> MgWO <sub>8</sub> ).				62Z1
4	Lattice distortion associated with the phase transition. Thermal expansion: Fig. 340.				62Z1
5a	Dielectric constants: Fig. 341, 342, 343. dΘ <sub>a</sub> /dp = -5.84 · 10 <sup>8</sup> °K N <sup>-1</sup> m <sup>2</sup> .				
6	Specific heat: Fig. 344. Transition heat (II → I): ΔQ <sub>m</sub> = 276 cal mol <sup>-1</sup> .				66S28
8a	Elastic compliance: Fig. 345. Ultrasound absorption: Fig. 346, 347.				
Nr. 1B2-ii Pb(Cd <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>					
1a	Synthesis of Pb(Cd <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> was reported by BELYAEV et al. in 1963.				63B3
b	phase	II	I		65F4
	state	(A)	P		
	crystal system	monoclinic	cubic		
	Θ	400 °C			
	a = (4.156 ± 0.002) Å, b = (4.074 ± 0.002) Å, β = 91° 9' ± 5' at RT. ROGINSKAYA and VENEVTSEV reported that another transition exists at 120 °C, in addition to the transition at 400 °C.				
3	Crystal structure: Superstructure lines, indicating ordered location of the octahedral voids of the perovskite lattice, were observed.				65R4
4	Lattice distortion: Fig. 348, 349.				65F4
5a	Dielectric constant: Fig. 350.				

Perovskite Types

Nr. 1B2-iii $\text{Pb}(\text{Mn}_{1/2}\text{W}_{1/2})\text{O}_3$						
1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by VENEVTSEV et al.					64V3
b	phase	II		I		65R5
	state	(A), $P_{\text{magn}}$		P, $P_{\text{magn}}$		
	crystal system	monoclinic		cubic		
	$\Theta$	423		$^{\circ}\text{K}$		
	$a = 4.063 \text{ \AA}$ , $b = 4.033 \text{ \AA}$ , $\beta = 90^{\circ} 12'$ at RT.					
5a	Dielectric constant: Fig. 351.					65R5
10	Electrical conductivity: $\sigma = 8 \cdot 10^{-8} \Omega^{-1} \text{ m}^{-1}$ .					65R5
11	Magnetic susceptibility: see Fig. 351.					
Nr. 1B2-iv $\text{Pb}(\text{Co}_{1/2}\text{W}_{1/2})\text{O}_3$						
1a	Antiferro- and ferroelectric properties in $\text{Pb}(\text{Co}_{1/2}\text{W}_{1/2})\text{O}_3$ were discovered by FILIP'EV et al.					63F1
b	phase	IV		III		65B8
	state	F, $F_{\text{magn}}$ (weak)		F, $P_{\text{magn}}$		a) 66K6
	crystal system			orthorhombic		b) 64F4
	$\Theta$	9a)		83 ... 103		293b)
	$a = 4.008 \text{ \AA}$ at 298 $^{\circ}\text{K}$ .					305
2a	Crystal growth: Flux method with $\text{PbO}$ .					65B8
3	Crystal structure: A superstructure was observed which was completely explained by alternation of the population of the oxygen octahedra by $\text{Co}^{2+}$ and $\text{W}^{6+}$ cations along the three directions. The real elementary lattice is a cubic face centered one with the parameter $A = 2a$ for phase I and with the parameters $A = 2 \cos(\beta/2)$ , $B = 2b$ , and $C = 2a \sin(\beta/2)$ for II, where $a$ , $b$ and $\beta$ are the parameters of the perovskite sublattice.					64F4
4	phase	lattice parameters				64F4
	I	$A = 8.017 \text{ \AA}$ at 298 $^{\circ}\text{K}$				
	II	$A = 5.669 \text{ \AA}$ , $B = 7.956 \text{ \AA}$ , $C = 5.689 \text{ \AA}$ at 258 $^{\circ}\text{K}$				
	Lattice distortion: Fig. 352.					
5a	Dielectric constant: Fig. 353, 354, 355.					
c	Polarization: Fig. 356.					
11	Magnetic susceptibility and magnetization: Fig. 357, 358.					
Nr. 1B2-v $\text{Pb}(\text{Mn}_{1/2}\text{Re}_{1/2})\text{O}_3$						
1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{Re}_{1/2})\text{O}_3$ was reported by VENEVTSEV et al.					64V3
b	phase	III		II		65R5
	state	(A), $F_{\text{magn}}$		(A), $P_{\text{magn}}$		
	crystal system			monoclinic		
	$\Theta$	103		393		
	$a = 4.043 \text{ \AA}$ , $b = 4.012 \text{ \AA}$ , $\beta = 90^{\circ} 33'$ at RT.					
3	Crystal structure: Ordered perovskite.					65R5

4	
10	
11	
Nr. 1	
1a	
b	
3	
5a	
c	
Nr. 1	
1a	
Nr. 1	
1a	
b	
2a	
3	
5a	
9a	
11	
12b	
c	

4	Lattice distortion: Fig. 359.			65R5
10	Electrical conductivity: $\sigma = 1 \cdot 10^{-1} \Omega^{-1} \text{ m}^{-1}$ .			65R5
11	Magnetic susceptibility and magnetic moment: Fig. 360. The linear temperature dependence of $\chi_{\text{magn}}^{-1}$ with a positive value of $\Theta_{\text{pmagn}} = 85^\circ\text{K}$ , and the appearing of the spontaneous moment at $103^\circ\text{K}$ , may indicate the presence of ferromagnetic properties in this compound, which is in agreement with the positive sign of the indirect exchange interaction proposed by GOODENOUGH for $\text{Mn}^{2+}$ and $\text{Re}^{6+}$ ions. However, the magnitudes of the calculated theoretical spontaneous moments agree with the experimental values only on the assumption of an anti-ferromagnetic interaction between ions distributed in an ordered fashion over the octahedral vacancies.			65R5
Nr. 1B3-i $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$				
1a	Ferroelectricity in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.			59S9
b	phase	II	I	59S9
	state	F	P	
	crystal system	tetragonal <sup>a)</sup> (possibly)	cubic	
	$\Theta$	90 $^\circ\text{C}$		
	$a = (4.074 \pm 0.001) \text{ \AA}$ , $c = (4.083 \pm 0.001) \text{ \AA}$ at RT. <sup>a)</sup>			
3	Crystal structure: In the powder patterns, additional to the principal lines of the perovskite structure, superstructural lines were observed indicating a doubling of the lattice period.			59I3
5a	Dielectric constant: Fig. 361.			59S9
c	Spontaneous polarization: $P_s \approx 3.6 \cdot 10^{-2} \text{ cm}^{-2}$ at $18^\circ\text{C}$ .			
Nr. 1B3-ii $\text{Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$				
1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$ with perovskite structure was reported by VENEVTSEV et al.			64V3
Nr. 1B3-iii $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$				
1a	Ferroelectricity in $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1958.			58S4
b	phase	III	II	62B7
	state	F, $A_{\text{magn}}$	F, $P_{\text{magn}}$	
	crystal system	rhombohedral	rhombohedral	
	space group		$\text{Pm}\bar{3}\text{m-O}_h^1$	
	$\Theta$	143 387 $^\circ\text{K}$		
	$a = 4.014 \text{ \AA}$ , $\alpha = 89.92^\circ$ at RT.			62B10
2a	Crystal growth: Flux method with $\text{PbO}$ .			62B7
3	Crystal structure: Disordered perovskite; X-ray studies have not shown any ionic ordering in the octahedral sites of perovskite structure. The magnetic peak was found in the neutron diffraction experiments at $78^\circ\text{K}$ . The effective magnetic moment of the $\text{Fe}^{3+}$ ion was found to be $(0.80 \pm 0.16) \mu_B$ at $78^\circ\text{K}$ from the calculation of the intensity of the (111) reflection, which is about 90% of the magnetic moment at $0^\circ\text{K}$ . Fig. 362.			64S8 65D6
5a	Dielectric constant: Fig. 363.			
9a	Optical absorption: Fig. 364.			
11	Magnetic susceptibility: Fig. 365. $\mu_{\text{eff}} = 5.4 \mu_B$ .			62B7
12b	ESR: Fig. 366.			66S22
c	Mössbauer effect: Fig. 367, 368. The quadrupile splitting $\Delta E_{\text{qu}} = (0.37 \pm 0.02) \text{ mm sec}^{-1}$ , the isomer shift $\delta = (0.52 \pm 0.02) \text{ mm sec}^{-1}$ , corresponding to trivalent iron (at $20^\circ\text{C}$ ).			





1b	phase	II	I	65K9	
	state	(A)	P		
	crystal system	monoclinic	cubic		
	$\Theta$	270 °C			
	$a = 4.152 \text{ \AA}$ , $b = 4.093 \text{ \AA}$ , $\beta = 90^\circ 30'$ at RT.				
4	Thermal expansion: Fig. 374.				
5a	Dielectric constant: Fig. 375.				
Nr. 1B3-x $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$					
1a	Ferroelectricity in $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was discussed by SMOLENSKII et al. in 1959.			59S9	
b	phase	II	I	59S9 *)59I3	
	state	F	P		
	crystal system	tetragonal*) (possibly)	cubic		
	$\Theta$	26 °C			
	$a = (4.072 \pm 0.001) \text{ \AA}$ , $c = (4.072 \pm 0.001) \text{ \AA}$ at RT*).				
3	Crystal structure: The large number of superstructure lines and their great intensity in $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ indicates that the degree of ordering of $\text{Sc}^{3+}$ and $\text{Ta}^{5+}$ ions is greater than in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$ . See 1B3-i-3.			59I3	
5a	Dielectric constant: Fig. 376.				
Nr. 1B3-xi $\text{Pb}(\text{Mn}_{1/2}\text{Ta}_{1/2})\text{O}_3$					
1a	$\text{Pb}(\text{Mn}_{1/2}\text{Ta}_{1/2})\text{O}_3$ with perovskite structure was synthesized by the addition of 5 mol% SrO.			65S17	
Nr. 1B3-xii $\text{Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$					
1a	Ferroelectricity in $\text{Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.			59S7	
b	phase	III	II	I	68N1 *)65S17
	state	F, $A_{\text{magn}}$	F, $P_{\text{magn}}$	P, $P_{\text{magn}}$	
	crystal system	rhombohedral	rhombohedral*)	cubic	
	space group			$\text{Pm}3\text{m}-O_h^h$	
	$\Theta$	143, 133*)	243, 233*)	°K	
	$P_s \parallel [111]$ (probably). $a = (4.007 \pm 0.001) \text{ \AA}$ at RT. black (dark orange for thin samples).				
2a	Crystal growth: Flux method with PbO. When the soak temperature is higher than 1200 °C, crystals are obtained having both pyrochloride and perovskite structure.			68N1	
3	Crystal structure: Disordered perovskite.			65S17	
4	phase	lattice constants		68N1	
	I	$a = (4.007 \pm 0.001) \text{ \AA}$ at RT.			
	II	$a = (4.006 \pm 0.001) \text{ \AA}$ at 90 °K $\alpha = 89.89^\circ \pm 0.02^\circ$			
5a	Dielectric constant: Fig. 377, 378.				
c	Spontaneous polarization: Fig. 379.				
11	Magnetic susceptibility: Fig. 380. $\mu_{\text{eff}} = 5.92 \mu_B$ ; $\Theta_{\text{p magn}} = -370 \text{ °K}$ .			68N1	



2a	Crystal growth: Flux method (using PbO). Kyropoulos method.	59M5 67B18															
3	Crystal structure: Disordered perovskite.	61B5															
4	Thermal expansion: Fig. 386.																
5a	Dielectric constant: Fig. 387, 388, 389.																
b	Nonlinear dielectric properties: $E = [(T - \Theta_p)(\epsilon_0 C)^{-1}] P + \xi P^3 + \zeta P^5 + \dots$ , where $\Theta_p = 265^\circ\text{K}$ , $C = (3.7 \pm 1.0) \cdot 10^8^\circ\text{K}$ , and $\xi \cong 5.6 \cdot 10^8 \text{ V m}^5 \text{ C}^{-2}$ .	67B9															
c	Spontaneous polarization and coercive field: Fig. 390.																
7a	Piezoelectricity: Fig. 391.																
9a	Refractive index: $n = 2.56$ for $6328 \text{ \AA}$ at $299^\circ\text{K}$ . Birefringence: It was found that the crystals $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ behave like optically isotropic crystals. An applied electric field causes double refraction. Fig. 392.	67B9															
c	Quadratic electrooptic effect: $M_{11} - M_{12} = +0.015 \text{ m}^4 \text{ C}^{-2}$ , $M_{44} = +0.008 \text{ m}^4 \text{ C}^{-2}$ for $6328 \text{ \AA}$ at $299^\circ\text{K}$ .	67B9															
14a	Domain structure: Clear domains were observed only in very thin wafers (e. g., $20 \cdot 10^{-6} \text{ m}$ ).	61B5															
<b>Nr. 1B4-ii <math>\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3</math></b>																	
1a	Ferroelectric $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ crystal was synthesized by Bokov and MYL'NIKOVA in 1960.	60B7															
b	<table border="1"> <tr> <td>phase</td><td>II</td><td>I</td></tr> <tr> <td>state</td><td>F</td><td>P</td></tr> <tr> <td>crystal system</td><td></td><td>cubic</td></tr> <tr> <td><math>\Theta</math></td><td>140</td><td><math>^\circ\text{C}</math></td></tr> </table> <p><math>a = 4.04 \text{ \AA}</math> at RT. light yellow.</p>	phase	II	I	state	F	P	crystal system		cubic	$\Theta$	140	$^\circ\text{C}$	60B7			
phase	II	I															
state	F	P															
crystal system		cubic															
$\Theta$	140	$^\circ\text{C}$															
2a	Crystal growth: Flux method with PbO. The crystals were separated from the matrix solution by washing in acetic acid at RT for a long time.	60B7															
5a	Dielectric constant: Fig. 393.																
<b>Nr. 1B4-iii <math>\text{Pb}(\text{Cd}_{1/3}\text{Nb}_{2/3})\text{O}_3</math></b>																	
1b	Dielectric anomaly in $\text{Pb}(\text{Cd}_{1/3}\text{Nb}_{2/3})\text{O}_3$ was reported by VENEVTSEV et al. in 1966.	65T5, 66V5															
<b>Nr. 1B4-iv <math>\text{Pb}(\text{Co}_{1/3}\text{Nb}_{2/3})\text{O}_3</math></b>																	
1a	Ferroelectricity in $\text{Pb}(\text{Co}_{1/3}\text{Nb}_{2/3})\text{O}_3$ was found by Bokov and MYL'NIKOVA in 1960.	60B7															
b	<table border="1"> <tr> <td>phase</td><td>II</td><td>I</td></tr> <tr> <td>state</td><td>F</td><td>P</td></tr> <tr> <td>crystal system</td><td></td><td>cubic</td></tr> <tr> <td>space group</td><td></td><td><math>\text{Pm}3\text{m-O}_h^1</math></td></tr> <tr> <td><math>\Theta</math></td><td>-98</td><td><math>^\circ\text{C}</math></td></tr> </table> <p><math>a = 4.04 \text{ \AA}</math> at RT. brown.</p>	phase	II	I	state	F	P	crystal system		cubic	space group		$\text{Pm}3\text{m-O}_h^1$	$\Theta$	-98	$^\circ\text{C}$	60B7
phase	II	I															
state	F	P															
crystal system		cubic															
space group		$\text{Pm}3\text{m-O}_h^1$															
$\Theta$	-98	$^\circ\text{C}$															
2a	Crystal growth: Flux method with PbO.	60B7															
5a	Dielectric constant: Fig. 394.																

1B4-viii  $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$

1a	Ferroelectricity in $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$ was found by BOKOV and MYL'NIKOVA in 1960.			60B7
b	phase	II	I	60B7
	state	F	P	
	crystal system		cubic	
	space group		$\text{Pm}\bar{3}\text{m-O}_h^1$	
	$\Theta$	-140	$^{\circ}\text{C}$	
	$a = 4.01 \text{ \AA}$ at RT. brown.			
2a	Crystal growth: Flux method with $\text{PbO}$ .			60B7
3	Crystal structure: Disordered perovskite.			60B7
5a	Dielectric constant: Fig. 401.			

1B4-viii  $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$

Nr.

1a

b

2a

3

5a

Nr.

1a

b

5a

10

11

Nr.

1a

b

2a

5a

11

12b

1C

Nr.

1b

5a

6a

7a

Nr. 1B4-viii  $\text{Pb}(\text{Ni}_{1/3}\text{Ta}_{2/3})\text{O}_3$ 

1a	Ferroelectricity in $\text{Pb}(\text{Ni}_{1/3}\text{Ta}_{2/3})\text{O}_3$ was found by BOKOV and MYL'NIKOVA in 1960.			60B7
b	phase	II	I	60B7
	state	F	P	
	crystal system		cubic	
	space group		$\text{Pm}\bar{3}\text{m}-\text{O}_h^1$	
	$\Theta$	-180	°C	
	$a = 4.01 \text{ \AA}$ at RT. green.			
2a	Crystal growth: Flux method.			60B7
3	Crystal structure: Disordered perovskite.			60B7
5a	Dielectric constant: Fig. 402.			

Nr. 1B5-i  $\text{Pb}(\text{Mn}_{2/3}\text{W}_{1/3})\text{O}_3$ 

1a	Dielectric and magnetic anomalies in $\text{Pb}(\text{Mn}_{2/3}\text{W}_{1/3})\text{O}_3$ were reported by ROGINSKAYA et al. in 1965.			65R5
b	phase	III	II	I
	state	(A), ( $A_{\text{magn}}$ )	(A), $P_{\text{magn}}$	P, $P_{\text{magn}}$
	crystal system		monoclinic	cubic
	$\Theta$	203	473	°K
	$a = c = 4.098 \text{ \AA}$ , $b = 4.014 \text{ \AA}$ , $\beta = 90^\circ 23'$ at RT.			
5a	Dielectric constant: Fig. 403.			65R5
10	$\sigma = 2 \cdot 10^{11} \Omega^{-1} \text{ m}^{-1}$ .			
11	Magnetic susceptibility: see Fig. 403. $\Theta_{\text{p magn}} = -75^\circ \text{K}$ .			

Nr. 1B5-ii  $\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3$ 

1a	Ferroelectricity in $\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.			59S7
b	phase	III	II	I
	state	F, $A_{\text{magn}}$	P, $A_{\text{magn}}$	P, $P_{\text{magn}}$
	crystal system		cubic	cubic
	$\Theta$	178	363	°K
	$a = 4.02 \text{ \AA}$ at RT.			65R5
2a	Flux method (PbO).			62B7
5a	Dielectric constant: Fig. 404.			
11	Magnetic susceptibility: see Fig. 404. Magnetization is a linear function of the magnetic field intensity up to 8000 Oe. Effective magnetic moment: $4.2 \mu_B$ .			62B7
12b	ESR: Fig. 405.			

## 1C Solid solutions with perovskite-type oxides as end members

Nr. 1C-a1  $\text{NaNbO}_3\text{-KNbO}_3$ 

1b	Phase diagram: Fig. 406, 407, 408. Lattice parameters: Fig. 409.	
5a	Dielectric constant: Fig. 410; see Tab. 60. Polarization and coercive field: Fig. 411.	
6a	Transition energy: Tab. 59.	
7a	Electromechanical properties: Fig. 412 ... 417; Tab. 60.	

Tab. 59.  $(\text{Na}_{1-x}\text{K}_x)\text{NbO}_3$ . Transition energy  $\Delta Q_m$ . [54S3]

$x$	Lower phase change	Upper phase change
1.00 ( $\text{KNbO}_3$ )	85 cal/mole	190 cal/mole
0.10	20 cal/mole	60 cal/mole
0 ( $\text{NaNbO}_3$ )	—	50 cal/mole

Tab. 60.  $(\text{Na}_{0.5}\text{K}_{0.5})\text{NbO}_3$  (ceramics). Electric and electromechanical constants. [59E1]

Dielectric constant (100 kHz)	290
Dissipation factor (100 kHz)	$\approx 4.0\%$
Specific resistivity $\rho$	$10^{10} \Omega \text{m}$
Density $\rho$	$4.25 \cdot 10^3 \text{ kg m}^{-3}$
Poisson's ratio (assumed)	0.27
Coupling factor $k_p$	$0.34 \dots 0.39$
Frequency constant $f_R$	1.67 kHz m
Mechanical $Q_{\text{mech}}$ (radial)	130
Young's modulus $E$	$1.04 \cdot 10^{11} \text{ N m}^{-2}$
Piezoelectric constant $-d_{31}$	$32 \cdot 10^{-12} \text{ C N}^{-1}$
Piezoelectric constant $-g_{31}$	$12.6 \cdot 10^{-3} \text{ m}^2 \text{ C}^{-1}$
Piezoelectric constant $d_{33}^*$	$80 \cdot 10^{-12} \text{ C N}^{-1}$
Piezoelectric constant $g_{33}^*$	$31.5 \cdot 10^{-3} \text{ m}^2 \text{ C}^{-1}$
Coupling factor $k_{33}^*$	0.51

Nr. 1C-a2  $\text{NaNbO}_3$ - $\text{NaTaO}_3$ 

1b	Phase diagram: Fig. 418. Lattice parameters: Fig. 419.
4	Thermal expansion: Fig. 420.
5a	Dielectric constant: Fig. 421.
9a	Birefringence: Fig. 422.

Nr. 1C-a3  $\text{NaNbO}_3$ - $\text{NaSbO}_3$ 

1a	Curie temperature: Fig. 423.
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Nr. 1C-a4  $\text{KNbO}_3$ - $\text{KTaO}_3$ 

1	Phase diagram: Fig. 424, 425.
5a	Dielectric properties: Fig. 426, 427. $\Theta_f$ : see Tab. 61.
6	Thermal properties: Fig. 428; Tab. 61.
9	See 1C-a5 for optical properties of $\text{K}(\text{Ta}_{0.35}\text{Nb}_{0.65})\text{O}_3$ (KTN).

Tab. 61.  $\text{K}(\text{Nb}_{1-x}\text{Ta}_x)\text{O}_3$ .  $L$ : latent heat,  $\Theta_f$ : Curie point,  $A$ : constant in the formula for free energy =  $A(T - \Theta_f)P^2 + \dots$ ,  $P_{\text{calc}}$ :  $P_s$  calculated for  $T = \Theta_f$ . [59H1]

$x$	$L$ cal mol $^{-1}$	$\Theta_f$ °K	$A$ $10^5 \text{ °K}^{-1}$	$P_{\text{calc}}$ $10^{-2} \text{ C m}^{-2}$
0	$110 \pm 10$	679	2.6	27
0.06	$46 \pm 4$	656	2.7	17.7
0.12	$10 \pm 2$	623	2.85	7.9
0.18	$4.0 \pm 2$	591	3.05	5.1

Nr. 1C-a5  $\text{K}(\text{Ta}_{0.35}\text{Nb}_{0.65})\text{O}_3$  (KTN)For general properties of  $\text{KNbO}_3$ - $\text{KTaO}_3$  see 1C-a4.

9b	Electroreflectance: Fig. 429.
d	Faraday rotation: Fig. 430. See also Tab. 44.

Nr. 1C-a6  $\text{CaTiO}_3$ - $\text{SrTiO}_3$ 

1b	Phase diagram: Fig. 431, 432, 433. Lattice parameters: Fig. 434.
5a	Dielectric constant: Fig. 435, 436.
c	Spontaneous polarization: Fig. 437.

Nr. 1C-a7  $\text{CaTiO}_3$ - $\text{BaTiO}_3$ 

1b	Phase diagram: Fig. 438, 439, 440. Lattice parameters: Fig. 441.
5a	Dielectric constant: Fig. 442, 443.
6b	Thermal conductivity: Fig. 444.
7a	Electromechanical property: Tab. 62. See Fig. 183 and Tab. 40.

\* Estimated values.

Tab. 62.  $(\text{Ba}_{1-x}\text{Ca}_x)\text{TiO}_3$  (ceramics, pure  $\text{BaTiO}_3$  base).  $d_{31}$  and  $d_{33}$  at RT. [57B4]

$x$	$\rho$ $10^3 \text{ kg m}^{-3}$	$\rho_x$ $10^3 \text{ kg m}^{-3}$	$d_{31}$ $10^{-12} \text{ C N}^{-1}$	$d_{33}$ $10^{-12} \text{ C N}^{-1}$	$-d_{33}/d_{31}$	Porosity ( $1 - (\rho/\rho_x)$ )
0	5.85	6.017	-97.5	229	2.35	0.028
0.05	5.70	5.85	-66.6	167	2.51	0.026
0.07	5.68	5.80	-58.0	150	2.58	0.021
0.09	5.65	5.74	-52.1	139	2.67	0.016
0.12	5.55	5.66	-43.4	124.5	2.88	0.019

Nr. 1C-a8  $\text{CaTiO}_3\text{-PbTiO}_3$ 1b | Curie temperature: Fig. 445.  
Lattice parameter: Fig. 446.Nr. 1C-a9  $\text{SrTiO}_3\text{-BaTiO}_3$ 1b | Phase diagram: Fig. 447 ... 450.  
Lattice parameter: Fig. 451; see Fig. 448.5a | Dielectric constant: Fig. 452.  
Microwave dielectric loss: Tab. 63.

6a | Specific heat: Fig. 453.

10b | Conductivity associated with doping: Fig. 454, 455, 456.

Tab. 63.  $(\text{Ba}_{1-x}\text{Sr}_x)\text{TiO}_3$ . Dielectric loss:  $\alpha, \beta, \gamma$  at 20 GHz. [62R4].  $(T - \Theta_p) \tan \delta = \alpha + \beta T + \gamma T^2$ .

Sample		Heat treatment	Grain size $\mu$	$\Theta_p$ $^\circ\text{K}$	$\alpha$ $^\circ\text{K}$	$\beta \cdot 10^4$	$\gamma \cdot 10^6$ ( $^\circ\text{K}$ ) $^{-1}$
Polycrystalline	$\text{SrTiO}_3$	Hot pressed and fired in air at 900 $^\circ\text{C}$ for 10 h	1	37	0.33	7.7	4.3
		Refired at 1200 $^\circ\text{C}$ in air for 10 h	3	37	0.26	5.5	4.7
		Refired at 1400 $^\circ\text{C}$ in air for 10 h	15	37	0.17	4.4	4.2
		Refired at 1500 $^\circ\text{C}$ in $\text{O}_2$ for 6 h	30	37	0.08	4.5	3.7
	$\text{Ba}_{0.2}\text{Sr}_{0.8}\text{TiO}_3$	Hot pressed and fired in $\text{O}_2$ at 1500 $^\circ\text{C}$ for 10 h	30	105	0.6	9	2.5
	$\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$	Hot pressed and fired in $\text{O}_2$ at 1500 $^\circ\text{C}$ for 10 h	30	218	2.0	(9) <sup>a)</sup>	(2.5)
	$\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$	Ceramic fired to 1375 $^\circ\text{C}$ in air for 1 h	8	280	2.2	(9)	(2.5)
	$\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$	Ceramic fired to 1300 $^\circ\text{C}$ in air for 1 h	8	324	1.6	(9)	(2.5)
Single crystal	$\text{SrTiO}_3$	None	$\infty$	37	0	6.53	2.54
	$\text{SrTiO}_3 + 0.1\% \text{ Gd}^{3+}$	None	$\infty$	37	0.033	(6.53)	(2.54)
	$\text{SrTiO}_3 + 0.03\% \text{ Fe}^{3+}$	None	$\infty$	37	0.043	(6.53)	(2.54)

Nr. 1C-a10  $\text{SrTiO}_3\text{-PbTiO}_3$ 1b | Curie temperature: Fig. 457.  
Lattice parameter: Fig. 458.5a | Dielectric constant: Fig. 459.  
Curie constant: Fig. 460.

6a | Transition heat: Fig. 461.

Nr. 1C-a11  $\text{BaTiO}_3\text{-PbTiO}_3$ 1b | Phase diagram: Fig. 462.  
Lattice parameter: Fig. 463.

5a | Dielectric constant: Fig. 464.

6a | Specific heat: Fig. 465.  
Transition heat: Fig. 466.

7 | Electromechanical properties: see 1A-8.

16 | Radiation damage: Fig. 467.

<sup>a)</sup> Values in parentheses indicate that these values were assumed in order to determine  $\alpha$ .



Nr. 1C-a12 $\text{CaZrO}_3\text{-BaZrO}_3$	1b   Lattice parameter: Fig. 468.
Nr. 1C-a13 $\text{CaZrO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 469.
	4   Thermal expansion: Fig. 470.
	5a   Dielectric constant: Fig. 471.
Nr. 1C-a14 $\text{SrZrO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 472, 473. Lattice parameter: Fig. 474.
	4   Thermal expansion: Fig. 475, 476, 477; Tab. 64.
	5a   Dielectric constant: Fig. 478, 479.
	c   Polarization: Fig. 480.
	6a   Specific heat: Fig. 481. Transition heat: Tab. 65.

Tab. 64.  $\text{PbZrO}_3$ ,  $(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$ , and  $(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$ .  $\Delta V/V$ .  $\Delta V$ : anomalous volume change at the transition point. [54S2]

Composition	$\Delta V/V [10^{-4}]$	
	Lowest phase	Intermediate phase
$\text{PbZrO}_3$	-41 at 230 °C	—
$(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$	-43 at 150 °C	+24 at 190 °C
$(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$	-30 at 210 °C	-20 at 230 °C

Tab. 65.  $\text{PbZrO}_3$ ,  $(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$ , and  $(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$ .  $\Delta Q_m$ . [52S2]

Composition	$\Delta Q_m [\text{cal mol}^{-1}]$	
	Lower transition	Upper transition
$\text{PbZrO}_3$	—	440
$(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$	190	230
$(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$	180	230

Nr. 1C-a15 $\text{BaZrO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 482. Lattice parameter: Fig. 483.
	4   Thermal expansion: Fig. 484.
	5a   Dielectric constant: Fig. 485 ... 488.
	c   Coercive field: Fig. 489.
	8   Elastic properties: Fig. 490.
Nr. 1C-a16 $\text{CaHfO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 491.
	5a   Dielectric constant: Fig. 492.
Nr. 1C-a17 $\text{SrHfO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 493.
	5a   Dielectric constant: Fig. 494.
Nr. 1C-a18 $\text{BaHfO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 495.
Nr. 1C-a19 $\text{CaSnO}_3\text{-SrSnO}_3$	1b   Lattice parameter: Fig. 496.
Nr. 1C-a20 $\text{BaSnO}_3\text{-SrSnO}_3$	1b   Lattice parameter: see Fig. 496.
Nr. 1C-a21 $\text{BaSnO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 497.
	5a   Dielectric constant: Fig. 498.
Nr. 1C-a22 $\text{CaTiO}_3\text{-CaZrO}_3$	1b   Lattice parameter: Fig. 499.

Nr. 1C-a23 BaTiO <sub>3</sub> -BaZrO <sub>3</sub>	1b	Phase diagram: Fig. 500. Lattice parameter: Fig. 501.	
	2a	Phase diagram: Fig. 502.	
	5a	Dielectric constant: Fig. 503.	
	8a	Elastic property: Fig. 504	
Nr. 1C-a24 BaTiO <sub>3</sub> -BaHfO <sub>3</sub>	1b	Phase diagram: Fig. 505. Lattice parameter: Fig. 506.	
	5a	Dielectric constant: Fig. 507.	
Nr. 1C-a25 BaTiO <sub>3</sub> -BaSnO <sub>3</sub>	1b	Phase diagram: Fig. 508. See also	59I2
	2a	Phase diagram: Fig. 509.	
	4	Thermal expansion: Fig. 510.	
	5a	Dielectric constant: Fig. 511.	
Nr. 1C-a26 BaTiO <sub>3</sub> -BaUO <sub>3</sub>	1b	Lattice parameter: Fig. 512.	
Nr. 1C-a27 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> Pb(Zr <sub>x</sub> Ti <sub>1-x</sub> )O <sub>3</sub> with $x = 0.5 \dots 0.6$ ; for electromechanical properties of these very important piezo-electric materials, see 1C-a28.			
1a	Ferro- and antiferroelectric phase transitions in the PbTiO <sub>3</sub> -PbZrO <sub>3</sub> system were revealed in 1952 by SHIRANE, SUZUKI and TAKEDA.		52S6, 52S4, 52S3
b	Phase diagram at high temperature: Fig. 513. Phase diagram: Fig. 514, 515. Lattice parameter: Fig. 516, 517.		
2	Flux method:		62I1, 64F6, 67F7
4	Lattice distortion: Fig. 518a, b, 519. Thermal expansion: Fig. 520, 521, 522.		
5a	Dielectric constant: Fig. 523 ... 526.		
c	Spontaneous polarization: Fig. 527. Critical field: Fig. 528.		
6	Specific heat: Fig. 529, 530. Transition energy: Tab. 66.		
7 } 8 }	Electromechanical properties: see 1C-a28.		
9	Birefringence: Fig. 531a, b, c.		
16	Radiation damage: Fig. 532.		

Tab. 66. Pb(Zr-Ti)O<sub>3</sub>. Transition energy and entropy. [53S1].  $x$ : atomic percent of PbTiO<sub>3</sub>;  $d\Theta/dx$ : shift of the transition temperature with  $x$ ;  $dS(d\Theta/dx)$ : it may be assumed that the free energy should decrease with the rate of  $dS(d\Theta/dx)$  with increasing  $x$ .

Kind of the phase change	$\Theta$ °C	$\Delta Q_m$ cal mol <sup>-1</sup>	$\Delta S_m$ cal mol <sup>-1</sup> °K <sup>-1</sup>	$d\Theta/dx$	$dS(d\Theta/dx)$
$A_\alpha \rightarrow P_\alpha$	$230 > T > 225$	400	0.8	—	(-5.8)
$A_\alpha \rightarrow A_\beta$	225	110	0.22	-16	-3.5
$A_\beta \rightarrow P_\alpha$	230	290	0.58	-4	-2.3
$A_\alpha \rightarrow F_\alpha$	240	—	—	-19	—
$F_\alpha \rightarrow P_\alpha$	217	250	0.51	+ 1.0	+0.5
$A_\beta \rightarrow F_\alpha$	—	40	0.08	—	—

Nr. 1C-a28 Pb(Zr <sub>x</sub> Ti <sub>1-x</sub> )O <sub>3</sub> (x = 0.5 ... 0.6, lead zirconate-titanate)												
For general properties of PbTiO <sub>3</sub> -PbZrO <sub>3</sub> , see 1C-a27.												
1a	JAFPE, ROTH, and MARZULLO discovered the excellent piezoelectric performances of Pb(Zr-Ti)O <sub>3</sub> ceramics in 1954. PZT is the trade mark of this substance developed by Clevite Corporation, Cleveland, Ohio, USA.											54J1
5a	Dielectric constants: Fig. 533 and Fig. 539, 540, 541, 543, 544.											
7) 8)	Electromechanical properties (ceramics): Tab. 67; Fig. 534 ... 538; Tab. 68 ... 72; Fig. 539 ... 542; Tab. 73; Fig. 543 ... 554.											
10	Electrical conductivity: see For breakdown, see											63G1, 61S14 59G2
Tab. 67. Pb(Ti <sub>1-x</sub> Zr <sub>x</sub> )O <sub>3</sub> [x = 0.48 ... 0.60] (ceramics). Electromechanical constants at RT. [60B3]												
Zr/Ti atom ratio	k <sub>31</sub>	k <sub>p</sub>	k <sub>15</sub>	k <sub>33</sub>	κ <sub>11</sub> <sup>T</sup>	κ <sub>11</sub> <sup>S</sup>	κ <sub>33</sub> <sup>T</sup>	κ <sub>33</sub> <sup>S</sup> obs	κ <sub>33</sub> <sup>S</sup> calc			
48/52	0.170	0.289	0.408	0.435	663	551	666	540	537			
50/50	0.230	0.397	0.504	0.546	855	631	846	585	585			
52/48	0.313	0.529	0.694	0.670	1180	612	730	399	389			
54/46	0.280	0.470	0.701	0.626	990	504	450	253	268			
56/44	0.267	0.450	0.657	0.619	840	477	423	246	258			
58/42	0.254	0.428	0.646	0.607	751	437	397	243	246			
60/40	0.238	0.400	0.625	0.585	672	410	376	240	245			
	s <sub>11</sub> <sup>E</sup>	s <sub>11</sub> <sup>D</sup>	s <sub>33</sub> <sup>E</sup>	s <sub>33</sub> <sup>D</sup>	s <sub>44</sub> <sup>E</sup>	s <sub>44</sub> <sup>D</sup>	s <sub>66</sub>	s <sub>12</sub> <sup>E</sup>	s <sub>12</sub> <sup>D</sup>	s <sub>13</sub> <sup>E</sup>	s <sub>13</sub> <sup>D</sup>	Density ρ
	10 <sup>-12</sup> m <sup>2</sup> N <sup>-1</sup>											10 <sup>3</sup> kgm <sup>-3</sup>
48/52	10.8	10.5	10.9	8.83	28.3	23.6	28.3	-3.35	-3.66	-3.21	-2.40	7.59
50/50	12.4	11.7	13.3	9.35	32.8	24.5	32.9	-4.06	-4.72	-4.22	-2.60	7.55
52/48	13.8	12.4	17.1	9.35	48.2	25.0	38.4	-4.07	-5.38	-5.80	-2.56	7.55
54/46	11.6	10.7	14.8	9.0	45.0	22.9	29.9	-3.33	-4.24	-4.97	-2.68	7.62
56/44	11.0	10.2	14.0	8.65	39.8	22.6	28.4	-3.22	-4.01	-4.63	-2.57	7.59
58/42	10.5	9.85	12.8	8.10	37.7	21.9	27.1	-3.07	-3.75	-4.12	-2.33	7.64
60/40	10.4	9.75	12.05	7.92	36.9	22.5	26.7	-2.96	-3.55	-3.72	-2.17	7.60
	g <sub>31</sub>	g <sub>33</sub>	g <sub>15</sub>	g <sub>33</sub> - g <sub>31</sub>	d <sub>31</sub>	d <sub>33</sub>	d <sub>15</sub>	d <sub>33</sub> - d <sub>31</sub>	s <sub>33</sub> <sup>D</sup> + s <sub>11</sub> <sup>D</sup> - 2s <sub>13</sub> <sup>D</sup>			
	10 <sup>-3</sup> m <sup>2</sup> C <sup>-1</sup>				10 <sup>-12</sup> C N <sup>-1</sup>				10 <sup>-12</sup> m <sup>2</sup> N <sup>-1</sup>			
48/52	- 7.3	18.7	28.4	26.0	43.0	110	166	153	24.1			
50/50	- 9.35	23.1	33.2	32.4	70.0	173	251	243	26.2			
52/48	-14.5	34.5	47.2	49.0	93.5	223	494	316	26.9			
54/46	-15.1	38.1	50.3	53.2	60.2	152	440	212	25.1			
56/44	-14.5	37.8	48.0	52.3	54.3	142	357	196	24.0			
58/42	-13.9	36.7	48.8	50.6	48.9	129	325	178	22.6			
60/40	-13.3	35.2	49.3	48.5	44.2	117	293	161	22.0			
	Q <sub>mech</sub>	Q <sub>E</sub> (=1/ tan δ)	P	c <sub>33</sub> <sup>D</sup>	-s <sub>12</sub> <sup>E</sup> s <sub>11</sub> <sup>E</sup>	-s <sub>12</sub> <sup>D</sup> s <sub>11</sub> <sup>D</sup>	-s <sub>13</sub> <sup>E</sup> √s <sub>33</sub> <sup>E</sup> s <sub>11</sub> <sup>E</sup>	-s <sub>13</sub> <sup>D</sup> √s <sub>33</sub> <sup>D</sup> s <sub>11</sub> <sup>D</sup>				
			10 <sup>-2</sup> C m <sup>-2</sup>	10 <sup>10</sup> N m <sup>-2</sup>								
48/52	1170	380	17	14.0	0.310	0.349	0.296	0.250				
50/50	950	370	27	13.5	0.328	0.404	0.329	0.249				
52/48	860	360	36	13.4	0.295	0.434	0.376	0.238				
54/46	680	300	42.5	14.8	0.288	0.396	0.380	0.273				
56/44	490	190	48	15.3	0.293	0.394	0.373	0.274				
58/42	500	200	43	15.8	0.292	0.381	0.355	0.261				
60/40	600	210	33	15.6	0.285	0.365	0.332	0.247				

Tab. 68.  $(\text{Pb}_{1-x}\text{Sr}_x)(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$  and  $(\text{Pb}_{1-x}\text{Ca}_x)(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$  (modified ceramics). Effects of Ca and Sr on electromechanical properties. [59K4]

Intended composition	$\epsilon_a$ $10^3$ $\text{kgm}^{-3}$	$\kappa$ at 1 kHz	24 hours after poling						$\Theta_f$ $^\circ\text{C}$
			$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	$g_{31}$ $10^{-3}$ $\text{m}^2\text{C}^{-1}$	$(s_{11}^E)^{-1}$ $10^{10}$ $\text{Nm}^{-2}$	
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.40	736	544	0.5	0.48	71	14.7	7.67	385
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.39	707	542	0.4	0.47	69	14.4	7.76	
$\text{Pb}_{0.99}\text{Ca}_{0.01}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.42	729	624	0.5	0.49	77	13.9	7.89	
$\text{Pb}_{0.99}\text{Sr}_{0.01}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.42	755	584	0.6	0.49	75	14.5	7.68	
$\text{Pb}_{0.95}\text{Ca}_{0.05}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.26	832	973	0.5	0.44	88	10.2	7.62	
$\text{Pb}_{0.95}\text{Sr}_{0.05}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.47	920	1002	0.4	0.50	101	11.4	7.65	360
$\text{Pb}_{0.92}\text{Ca}_{0.08}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	6.86	794	888	0.4	0.32	60	7.6	7.85	
$\text{Pb}_{0.925}\text{Sr}_{0.075}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.29	942	1094	0.3	0.50	103	10.6	7.94	
$\text{Pb}_{0.90}\text{Sr}_{0.10}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.22	997	1129	0.3	0.49	103	10.3	7.95	290
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.47}\text{Ti}_{0.53})\text{O}_3$	7.09	609	663	0.3	0.28	40	6.8	9.91	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.50}\text{Ti}_{0.50})\text{O}_3$	7.11	813	880	0.3	0.33	57	7.3	9.05	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$	7.10	973	1149	0.3	0.44	91	9.0	8.32	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.14	1076	1237	0.4	0.47	100	9.1	8.06	265
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	7.16	1095	1325	0.6	0.51	119	10.1	7.51	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	7.14	1105	1210	0.4	0.51	116	10.8	7.31	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.59}\text{Ti}_{0.41})\text{O}_3$	7.17	919	585	0.4	0.45	66	12.7	8.39	
$\text{Pb}_{0.85}\text{Sr}_{0.15}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	6.90	1106	1260	0.5	0.43	97	8.7	7.68	242
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	6.56	941	970	0.6	0.29	56	6.5	8.11	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	6.48	1212	1257	0.5	0.34	86	7.8	7.05	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	6.36	1182	1341	0.8	0.35	91	7.7	6.18	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.55}\text{Ti}_{0.45})\text{O}_3$	6.36	1200	1337	0.8	0.34	86	7.3	6.42	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	6.35	1107	1113	0.7	0.35	81	8.2	6.50	

Tab. 69.  $\text{Pb}(\text{Zr-Ti})\text{O}_3$  (ceramics, modified). Electromechanical properties of  $\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$  with five-valent additives. [59K5].  $f_R \cdot r$ : radial frequency constant

Addition wt. %	$\epsilon_a$ $10^3$ $\text{kgm}^{-3}$	Before poling		24 hours after poling						$\Theta_f$ $^\circ\text{C}$
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ $\text{Hz} \cdot \text{m}$	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	$Q_{\text{mech}}$	
None	7.41	707	0.3	537	0.4	0.49	1641	71		390
None	7.29	706	0.4	513	0.5	0.50	1687	69		387
0.1 $\text{Nb}_2\text{O}_5$	7.26	598	0.3	508	0.4	0.38	1643	54		
0.5 $\text{Nb}_2\text{O}_5$	6.96	732	2.1	790	2.0	0.46	1443	94		
0.8 $\text{Nb}_2\text{O}_5$	7.36	965	1.6	1166	1.5	0.48	1606	105		
1.0 $\text{Nb}_2\text{O}_5$	7.36	1064	1.8	1308	1.6	0.53	1563	126	61	
1.0 $\text{Nb}_2\text{O}_5$	7.60	1055	2.2	1242	2.2	0.54	1538	125		361
1.2 $\text{Nb}_2\text{O}_5$	7.34	1011	2.0	1167	1.7	0.48	1614	104	70	
1.4 $\text{Nb}_2\text{O}_5$	7.37	1057	2.2	1218	1.9	0.50	1584	113	69	
1.7 $\text{Nb}_2\text{O}_5$	7.39	1058	2.0	1218	1.8	0.47	1594	105		
2.0 $\text{Nb}_2\text{O}_5$	7.37	1074	2.1	1202	2.0	0.50	1550	115		344
0.5 $\text{Nb}_2\text{O}_5$	7.39	1169	2.1	1377	2.0	0.57	1491	146	48	369
0.5 $\text{La}_2\text{O}_3$										
1.0 $\text{Ta}_2\text{O}_5$	7.31	989	1.5	1187	1.5	0.49	1563	111	61	
1.0 $\text{Ta}_2\text{O}_5$	7.22	918	2.0	1121	2.1	0.50	1525	114		368
2.0 $\text{Ta}_2\text{O}_5$	7.49	1062	2.2	1230	2.1	0.50	1547	115		
2.0 $\text{Ta}_2\text{O}_5$	7.40	1077	1.8	1275	1.8	0.48	1581	111		364
2.5 $\text{Ta}_2\text{O}_5$	7.23	959	2.7	1112	2.4	0.36	1518	82	28	
5.0 $\text{Ta}_2\text{O}_5$	6.75	995	2.5	1052	2.6	0.33	1508	76		

Tab. 70.  $\text{Pb}(\text{Zr-Ti})\text{O}_3$  (ceramics, modified). Electromechanical properties of  $\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$  with three-valent additives. [59K5].  $f_R \cdot r$ : radial frequency constant

Addition wt. %	$\epsilon_a$ $10^3$ $\text{kgm}^{-3}$	Before poling		24 hours after poling					$\Theta_r$ $^\circ\text{C}$
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ $\text{Hz} \cdot \text{m}$	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	
None	7.41	707	0.3	537	0.4	0.49	1641	71	390
None	7.29	706	0.4	513	0.5	0.50	1687	69	387
1.0 $\text{Y}_2\text{O}_3$	7.26	796	0.9	841	1.0	0.34	1547	66	374
1.0 $\text{La}_2\text{O}_3$	7.46	1187	1.9	1483	2.0	0.53	1510	138	
1.0 $\text{La}_2\text{O}_3$	7.47	1139	2.2	1387	2.1	0.52	1522	130	339
1.0 $\text{Nd}_2\text{O}_3$	7.43	1111	1.6	1395	1.8	0.49	1512	123	
1.0 $\text{Nd}_2\text{O}_3$	7.37	1101	1.9	1354	1.8	0.48	1511	119	348
1.0 didymia	7.41	1122	2.2	1341	2.2	0.50	1499	125	
2.0 $\text{La}_2\text{O}_3$	7.49	1296	2.6	1545	2.3	0.51	1545	132	
1.0 $\text{La}_2\text{O}_3$	7.20	1375	2.1	1792	1.7	0.51	1528	147	
1.0 $\text{Nd}_2\text{O}_3$	7.35	1362	2.2	1776	1.9	0.49	1558	136	
0.1 $\text{La}_2\text{O}_3$	6.75	790	0.4	870	0.6	0.42	1505	88	
0.2 $\text{La}_2\text{O}_3$	6.45	686	0.7	735	0.9	0.37	1419	78	
0.4 $\text{La}_2\text{O}_3$	6.44	942	1.4	1100	1.5	0.42	1407	109	
0.8 $\text{La}_2\text{O}_3$	7.19	1288	1.8	1682	1.8	0.49	1516	139	
1.0 $\text{La}_2\text{O}_3$	7.50	1255	2.4	1532	2.4	0.50	1550	128	

Tab. 71. Electromechanical properties of  $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$  (ceramics), modified with additives of 1 wt% Nb. [59K5].  $f_R \cdot r$ : radial frequency constant

Base composition	$\epsilon_a$ $10^3$ $\text{kgm}^{-3}$	Before poling		24 hours after poling					
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ $\text{Hz} \cdot \text{m}$	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	$Q_{\text{mech}}$
$\text{Pb}(\text{Zr}_{0.50}\text{Ti}_{0.50})\text{O}_3$	7.38	879	1.5	1041	1.2	0.42	1696	82	81
$\text{Pb}(\text{Zr}_{0.51}\text{Ti}_{0.49})\text{O}_3$	7.31	975	1.6	1188	1.3	0.45	1642	97	73
$\text{Pb}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$	7.39	985	1.5	1200	1.4	0.45	1640	97	76
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.43	1092	1.8	1371	1.4	0.53	1547	130	61
$\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	7.44	1051	1.8	1296	1.7	0.54	1549	128	62
$\text{Pb}(\text{Zr}_{0.55}\text{Ti}_{0.45})\text{O}_3$	7.40	955	2.4	973	2.0	0.56	1524	117	55
$\text{Pb}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	7.38	818	2.8	745	2.5	0.53	1601	93	56
$\text{Pb}(\text{Zr}_{0.57}\text{Ti}_{0.43})\text{O}_3$	7.41	750	3.0	684	2.5	0.50	1636	82	60
$\text{Pb}(\text{Zr}_{0.58}\text{Ti}_{0.42})\text{O}_3$	7.41	713	3.0	630	2.8	0.49	1676	75	62

Tab. 72. Electromechanical properties of  $(\text{Pb}_{0.95}\text{Sr}_{0.05})(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$  (ceramics) with  $\text{Nb}_2\text{O}_5$  or  $\text{Ta}_2\text{O}_5$ . [59K5].  $f_R \cdot r$ : radial frequency constant

Addition wt. %	$\epsilon_a$ $10^3$ $\text{kgm}^{-3}$	Before poling		24 hours after poling					$\Theta_r$ $^\circ\text{C}$
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ $\text{Hz} \cdot \text{m}$	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	
1.0 $\text{Nb}_2\text{O}_5$	7.34	1291	2.0	1609	2.0	0.56	1512	153	306
2.0 $\text{Nb}_2\text{O}_5$	7.22	1380	2.4	1662	2.1	0.47	1562	127	
3.0 $\text{Nb}_2\text{O}_5$	6.63	1125	2.1	1301	2.1	0.36	1550	91	
2.0 $\text{Ta}_2\text{O}_5$	7.33	1343	2.3	1695	2.0	0.54	1517	151	296

ith	$\theta_r$ °C	$r$ Ta <sub>2</sub> O <sub>5</sub>	$\theta_r$ °C	% Nb.	$Q_{mech}$	81 73 76 61 62 55 56 60 62
	306					
	296					

Tab. 73. PZT (commercial modified ceramics). Electromechanical constants at RT. [66b7]

Substance	$\kappa_{11}^T$	$\kappa_{11}^S$	$\kappa_{33}^T$	$\kappa_{33}^S$	$10^{-12} \text{ C N}^{-1}$			$\text{C m}^{-2}$			$10^{-3} \text{ m}^2 \text{ C}^{-1}$			$h_{15}$ $10^8 \text{ N C}^{-1}$
					$d_{15}$	$d_{31}$	$d_{33}$	$e_{15}$	$e_{31}$	$e_{33}$	$g_{15}$	$g_{31}$	$g_{33}$	
PZT-2	990	504	450	260	440	-60.2	152	9.8	-1.86	9.0	50.3	-15.1	38.1	21.9
PZT-4	1475	730	1300	635	496	-123	289	12.7	-5.2	15.1	39.4	-11.1	26.1	19.7
PZT-5A	1730	916	1700	830	584	-171	374	12.3	-5.4	15.8	38.2	-11.4	24.8	15.2
PZT-5H	3130	1700	3400	1470	741	-274	593	17.0	-6.55	23.3	26.8	-9.11	19.7	11.3
PZT-6A			1100			-77	195					-7.9	17.0	
PZT-6B	515	441	500	420	135	-29	76	4.8	-0.96	7.4	29.6	-6.6	17.3	12.2
PZT-7A	840	450	425	235	368	-61	153	9.3	-2.15	9.7	49.5	-16.2	40.7	23.4
PZT-8			1000			-95	215					-10.5	24.5	
	$h_{31}$	$h_{33}$	$k_{15}$	$k_{31}$	$k_{33}$	$k_p$	$s_{11}^E$	$s_{11}^D$	$s_{33}^E$	$s_{33}^D$	$s_{12}^E$	$s_{12}^D$	$s_{13}^E$	$s_{13}^D$
PZT-2	-8.1	39.2	0.701	0.28	0.626	0.47	11.6	10.7	14.8	9.0	-3.33	-4.24	-4.97	-2.68
PZT-4	-9.2	26.8	0.71	0.334	0.70	0.58	12.3	10.9	15.5	7.90	-4.05	-5.42	-5.31	-2.10
PZT-5A	-7.3	21.5	0.685	0.344	0.705	0.60	16.4	14.4	18.8	9.46	-5.74	-7.71	-7.22	-2.98
PZT-5H	-5.05	18.0	0.675	0.388	0.752	0.65	16.5	14.05	20.7	8.99	-4.78	-7.27	-8.45	-3.05
PZT-6A				0.229	0.54	0.39	11.5	10.9			-3.45	-4.05		
PZT-6B	-2.6	19.9	0.377	0.145	0.375	0.25	9.0	8.8	9.35	8.05	-3.0	-3.2	-3.1	-2.6
PZT-7A	-10.4	46.6	0.68	0.306	0.67	0.52	10.7	9.7	13.9	7.65	-3.2	-4.2	-4.6	-2.3
PZT-8				0.295	0.60	0.50	11.1	10.1	13.9	8.9				
	$s_{44}^E$	$s_{44}^D$	$s_{66}$	$c_{11}^E$	$c_{11}^D$	$c_{33}^E$	$c_{33}^D$	$c_{12}^E$	$c_{12}^D$	$c_{13}^E$	$c_{13}^D$	$c_{44}^E$	$c_{44}^D$	$c_{66}$
$10^{-12} \text{ m}^2 \text{ N}^{-1}$														
PZT-2	45.0	22.9	29.9	135	136	113	148	67.9	69.3	68.1	61.2	22.2	43.7	33.4
PZT-4	39.0	19.3	32.7	139	145	115	159	77.8	83.9	74.3	60.9	25.6	51.8	30.6
PZT-5A	47.5	25.2	44.3	121	126	111	147	75.4	80.9	75.2	65.2	21.1	39.7	22.6
PZT-5H	43.5	23.7	42.6	126	130	117	157	79.5	82.8	84.1	72.2	23.0	42.2	23.5
PZT-6A			29.9											
PZT-6B	28.2	24.2	24.0	168	169	163	177	85.1	86.2	84.0	82.4	35.4	41.3	41.7
PZT-7A	39.5	21.2	27.8	148	157	131	175	76.2	85.4	74.2	73.0	25.3	47.2	36.0
PZT-8			29.6											

Nr. 1C-a29 $\text{PbTiO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 555, 556
Nr. 1C-a30 $\text{PbTiO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 557.
	5a   Dielectric constant: Fig. 558.
Nr. 1C-a31 $\text{PbZrO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 559.
Nr. 1C-a32 $\text{PbZrO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 560. Lattice parameter: Fig. 561.
	4   Thermal expansion: Fig. 562, 563.
	5a   Dielectric constant: Fig. 564a, b.
Nr. 1C-a33 $\text{LaFeO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 565. Lattice parameter: Fig. 566a, b.
	5a   Dielectric constant: Fig. 567.
	11   Magnetization: see Fig. 565.
Nr. 1C-b1 $\text{NaNbO}_3\text{-KTaO}_3$	1b   Phase diagram: Fig. 568. Lattice parameter: Fig. 569.
	4   Thermal expansion: Fig. 570.
	5a   Dielectric constant: Fig. 571.
Nr. 1C-b2 $\text{NaNbO}_3\text{-KSbO}_3$	1a   Curie temperature: see Fig. 423.
Nr. 1C-b3 $\text{BaTiO}_3\text{-PbZrO}_3$	4   Thermal expansion: Fig. 572.
	5a   Dielectric constant: Fig. 573.
Nr. 1C-b4 $\text{BaTiO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 574.
	5a   Dielectric constant: Fig. 575.
Nr. 1C-b5 $\text{PbTiO}_3\text{-CaZrO}_3$	1b   Phase diagram: Fig. 576. Lattice parameter: Fig. 577.
	5a   Dielectric constant: Fig. 578.
Nr. 1C-b6 $\text{PbTiO}_3\text{-CaSnO}_3$	1b   Phase diagram: see Fig. 576. Lattice parameter: Fig. 579.
	5a   Dielectric constant: Fig. 580.
Nr. 1C-b7 $\text{PbTiO}_3\text{-SrZrO}_3$	1b   Phase diagram: Fig. 581. Lattice parameter: Fig. 582a, b.
	5a   Dielectric constant: Fig. 583.
Nr. 1C-b8 $\text{PbTiO}_3\text{-SrSnO}_3$	1b   Phase diagram: Fig. 584. Lattice parameter: Fig. 585a, b.
	5a   Dielectric constant: Fig. 586.
Nr. 1C-b9 $\text{PbTiO}_3\text{-BaZrO}_3$	1b   Phase diagram: Fig. 587. Lattice parameter: Fig. 588a, b.
	5a   Dielectric constant: Fig. 589.
	7a   Electromechanical property: Tab. 74.

Tab. 74.  $(1-x)\text{PbTiO}_3 - x\text{BaZrO}_3$  (ceramics).  $k_p$  and  $d_{33}$  at RT. [63B15]

$x$	Poling field $\cdot 10^5 \text{ V m}^{-1}$ [ $T$ in $^\circ\text{C}$ ]	$k_p$	$d_{33}$ $\cdot 10^{-12} \text{ C N}^{-1}$
0.25	29 [185 ... 40]	0.16	40
0.30	27 [170 ... 40]	0.23	50
0.35	39 [145 ... 40]	0.30	110
0.40	30 [120 ... 40]	0.17	45

Nr. 1C-b10 $\text{PbTiO}_3\text{-BaSnO}_3$	1b   Phase diagram: Fig. 590. Lattice parameter: Fig. 591a, b.
Nr. 1C-b11 $\text{LaAlO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 592. Lattice parameter: Fig. 593. 5a   Dielectric constant: Fig. 594.
Nr. 1C-b12 $\text{LaCrO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 595. Lattice parameter: Fig. 596a, b. 4   Thermal expansion: Fig. 597. 11   Spontaneous magnetization: see Fig. 595.
Nr. 1C-c1 $\text{NaNbO}_3\text{-CaTiO}_3$	1b   Phase diagram: Fig. 598. 5a   Dielectric constant: Fig. 599.
Nr. 1C-c2 $\text{NaNbO}_3\text{-BaTiO}_3$	1b   Phase diagram: Fig. 600.
Nr. 1C-c3 $\text{NaNbO}_3\text{-PbTiO}_3$	1b   Transition temperature: Fig. 601. 5a   Dielectric constant: Fig. 602.
Nr. 1C-c4 $\text{NaNbO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 603. 5a   Dielectric constant: Fig. 604a, b.
Nr. 1C-c5 $\text{KNbO}_3\text{-BaTiO}_3$	1b   Phase diagram: Fig. 605. Lattice parameter: Fig. 606. 5a   Dielectric constant: Fig. 607a, b, c.
Nr. 1C-c6 $\text{KNbO}_3\text{-PbTiO}_3$	1b   Phase diagram: Fig. 608. Lattice parameter: Fig. 609. 5a   Dielectric constant: Fig. 610a, b.
Nr. 1C-c7 $\text{SrTiO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 611. Lattice parameter: Fig. 612. 5a   Relaxation phenomena are observed in the range II [65F1].
Nr. 1C-c8 $\text{BaTiO}_3\text{-LaAlO}_3$	1b   Lattice parameter and Curie temperature: Tab. 75.



Tab. 75. BaTiO<sub>3</sub>-LaAlO<sub>3</sub>. Lattice parameters and  $\Theta_r$ . [5814]

Concentration mol%		a Å	c Å	c/a	V Å <sup>3</sup>	$\Theta_r$ °C
BaTiO <sub>3</sub>	LaAlO <sub>3</sub>					
100.0	—	3.9956	4.0352	1.0100	64.42	+120
99.0	1.0	3.9951	4.0345	1.0098	64.39	+87
97.5	2.5	3.9949	4.0293	1.0086	64.30	+46
95.0	5.0	4.0050	—	1.0000	64.24	—14
92.5	7.5	4.0011	—	1.0000	64.05	—85
90.0	10.0	3.9984	—	1.0000	63.92	—133
87.5	12.5	3.9950	—	1.0000	63.76	—
85.0	15.0	3.9906	—	1.0000	63.55	—
75.0	25.0	3.9800	—	1.0000	63.04	—
—	100.0	3.7950	—	1.000	54.65	—

Nr. 1C-c9 BaTiO <sub>3</sub> -BiFeO <sub>3</sub>	11, 12	Néel temperature and magnetic resonance line width: Fig. 613.
Nr. 1C-c10 PbTiO <sub>3</sub> -LaAlO <sub>3</sub>	1b, 5a	Phase diagram: Fig. 614. Lattice parameter: Fig. 615. Dielectric constant: Fig. 616.
Nr. 1C-c11 PbTiO <sub>3</sub> -LaMnO <sub>3</sub>	1b	Transition temperatures: Fig. 617. Lattice parameters: Fig. 618.
Nr. 1C-c12 PbTiO <sub>3</sub> -LaFeO <sub>3</sub>	1b, 5a	Phase diagram: Fig. 619. Lattice parameter: Fig. 620. Dielectric constant: Fig. 621.
Nr. 1C-c13 PbTiO <sub>3</sub> -BiFeO <sub>3</sub>	1b, 4, 5a	Phase diagram: Fig. 622a, b. Lattice parameter: Fig. 623a, b. Thermal expansion: Fig. 624. Dielectric constant: Fig. 625.
Nr. 1C-c14 PbZrO <sub>3</sub> -BiFeO <sub>3</sub>	1b, 5a	Phase diagram: Fig. 626. Lattice parameter: Fig. 627. Dielectric constant: Fig. 628.
Nr. 1C-c15 SrSnO <sub>3</sub> -BiFeO <sub>3</sub>	1b, 12c	Phase diagram: Fig. 629. Mössbauer absorption: Fig. 630.
Nr. 1C-c16 SrFeO <sub>3</sub> -BiFeO <sub>3</sub>	1a, 11	Unit cell volume: Fig. 631. Magnetization: Fig. 632.
Nr. 1C-d1 SrTiO <sub>3</sub> -Sr(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1b	Phase diagram: Fig. 633.
Nr. 1C-d2 BaTiO <sub>3</sub> -Ba(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	2b	Phase diagram: Fig. 634.
Nr. 1C-d3 BaTiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1b	Curie temperature: Fig. 635. Lattice parameters: Fig. 636.
Nr. 1C-d4 PbTiO <sub>3</sub> -(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1b, 5a	Phase diagram and lattice parameters: Fig. 637. Dielectric constant: Fig. 638.
Nr. 1C-d5 PbTiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1b	Curie temperature and lattice parameters: Fig. 639.
Nr. 1C-d6 PbTiO <sub>3</sub> -(Li <sub>1/2</sub> La <sub>1/2</sub> )TiO <sub>3</sub>	1b	Curie temperature and lattice parameters: Fig. 640.

Nr. 1C-d7 $\text{PbTiO}_3\text{-(Na}_{1/2}\text{La}_{1/2})\text{TiO}_3$	1b   Curie temperature and lattice parameters: Fig. 641.
Nr. 1C-d8 $\text{PbTiO}_3\text{-(Li}_{1/2}\text{Ce}_{1/2})\text{TiO}_3$	1b   Lattice parameters: Fig. 642.
Nr. 1C-d9 $\text{PbTiO}_3\text{-(Li}_{1/2}\text{Nd}_{1/2})\text{TiO}_3$	1b   Lattice parameters: Fig. 643.
Nr. 1C-d10 $\text{PbTiO}_3\text{-Pb(Mg}_{1/2}\text{W}_{1/2})\text{O}_3$	1b   Phase diagram: Fig. 644. Lattice parameters: Fig. 645.
Nr. 1C-d11 $\text{PbTiO}_3\text{-Pb(Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1b   Curie temperature: Fig. 646.
Nr. 1C-d12 $\text{PbTiO}_3\text{-Pb(Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Curie temperature: Fig. 647.
Nr. 1C-d13 $\text{PbTiO}_3\text{-Pb(Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Transition temperature: Fig. 648. Lattice parameters: Fig. 649.
Nr. 1C-d14 $\text{PbZrO}_3\text{-Pb(Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Curie temperature: see Fig. 647.
Nr. 1C-d15 $\text{PbZrO}_3\text{-Pb(Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1b   Curie temperature: Fig. 650.
Nr. 1C-d16 $\text{PbZrO}_3\text{-(Na}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$	1b   Phase diagram: Fig. 651.
	4   Lattice distortion: Fig. 652.
	5a   Dielectric constant: Fig. 653.
Nr. 1C-d17 $\text{PbZrO}_3\text{-(K}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$	1b   Phase diagram: Fig. 654. Lattice parameters: Tab. 76.
	4   Lattice distortion: Fig. 655.
	5a   Dielectric constants: Fig. 656.

Tab. 76.  $(1-x)\text{PbZrO}_3-x(\text{K}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$ . Lattice constants at RT [62B10]

$x$	$a$ Å	$b$ Å	$c$ Å	
0	5.884	11.768	8.220	orthorhombic
0.10	5.882	11.764	8.227	orthorhombic
0.20	5.877	11.755	8.237	orthorhombic
0.30	5.876	11.751	8.248	orthorhombic
0.40	4.151	—	—	cubic
0.50	4.152	—	—	cubic

Nr. 1C-d18 $\text{PbHfO}_3\text{-Pb(Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Curie temperature: see Fig. 647.
Nr. 1C-d19 $\text{Pb(Mg}_{1/2}\text{W}_{1/2})\text{O}_3\text{-Pb(Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$	1b   Phase diagram: Fig. 657.
Nr. 1C-d20 $(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3\text{-(K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1b   Curie temperature: see Fig. 635. Lattice parameters: see Fig. 636.
Nr. 1C-d21 $\text{PbZrO}_3\text{-(Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1b   Phase diagram: Fig. 658. Lattice parameters: Fig. 659.
Nr. 1C-d22 $\text{BiFeO}_3\text{-Sr(Sn}_{1/3}\text{Mn}_{2/3})\text{O}_3$	1b   Phase diagram: Fig. 660. Lattice parameters: Fig. 661.
	12c   Mössbauer effect: see [65M8]
Nr. 1C-d23 $\text{BiFeO}_3\text{-Pb(Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Lattice parameters: Fig. 662.
	5a   Dielectric constant: Fig. 663.
	11   Magnetic susceptibility: Fig. 664. Néel temperature and spontaneous magnetization: Fig. 665.

Nr. 1C-e1 NaNbO <sub>3</sub> -LiNbO <sub>3</sub>	1b	Phase diagram: Fig. 666.
	5a	Dielectric constant: Fig. 667.
Nr. 1C-e2 NaNbO <sub>3</sub> -NaVO <sub>3</sub>	5a	Dielectric constant: Fig. 668.
	14b	Switching: see Fig. 9.
Nr. 1C-e3 NaNbO <sub>3</sub> -CaNb <sub>2</sub> O <sub>6</sub>	1b	Phase diagram: Fig. 669.
	5a	Dielectric constant: Fig. 670.
Nr. 1C-e4 NaNbO <sub>3</sub> -CdNb <sub>2</sub> O <sub>6</sub>	1b	Phase diagram: Fig. 671, 672. Lattice parameter: Fig. 673.
	5a	Dielectric constant: Fig. 674; Tab. 77.
	7a	Piezoelectricity: Fig. 675; Tab. 78.

Tab. 77. (1 - x)NaNbO <sub>3</sub> - (x/2)CdNb <sub>2</sub> O <sub>6</sub> [56L2]. r: capacitance ratio; C: Curie constant; Θ <sub>r</sub> , Θ compare Fig. 671, 672											
Composition x	Firing conditions			x <sub>RT</sub>	r	Θ °C	x <sub>max</sub>	Θ <sub>r</sub> °C	C · 10 <sup>4</sup> °C	Θ <sub>p</sub> °C	ρ 10 <sup>3</sup> kg m <sup>-3</sup>
	T °C	t hr	atmos- phere								
0.02	1250	1	CdO	230	—	200	2700	375	12	345	3.9
0.05	1250	1	CdO	500	1200	60	4000	375	12	345	4.2
0.10	1250	1	CdO	1000	130	75	4100	320	18	275	4.3
0.15	1250	1	CdO	1400	40	50	8500	285	24	260	4.3
0.20	1250	1	CdO	2300	20	20	10000	250	14	250	4.4
0.25	1250	1	CdO	3500	10	5	15000	220	20	230	4.5
0.30	1220	2	CdO	2700	12	-25	11000	210	20	205	4.6

Tab. 78. (1 - x)NaNbO <sub>3</sub> - (x/2)CdNb <sub>2</sub> O <sub>6</sub> (ceramics) [62K4]							
x	0.05	0.10	0.15	0.20	0.25	0.30	
ρ	4.2	4.3	4.3	4.3	4.4	4.2	10 <sup>3</sup> kg m <sup>-3</sup>
f <sub>R</sub> · 2r	3.0	3.0	3.0	3.15	3.36	3.25	10 <sup>3</sup> Hz m
s <sub>11</sub> <sup>E</sup>	11.9	11.6	11.6	10.5	9.0	10.1	10 <sup>-12</sup> m <sup>2</sup> N <sup>-1</sup>
tan δ	0.01	0.01	0.02	0.01	0.01	0.03	
x at Θ <sub>r</sub>	4	4.1	8.5	16	13	11	10 <sup>3</sup>

Nr. 1C-e5 NaNbO <sub>3</sub> -SrNb <sub>2</sub> O <sub>6</sub>	1b	Phase diagram: Fig. 676. Lattice parameter: Fig. 677.
	5a	Dielectric constant: Fig. 678.
	7a	Electromechanical properties: Fig. 679, 680, 681.
Nr. 1C-e6 NaNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1b	Phase diagram: Fig. 682. Lattice parameter: Fig. 683.
	7a	Electromechanical properties: Fig. 684.
Nr. 1C-e7 CdTiO <sub>3</sub> -LiNbO <sub>3</sub> , CdTiO <sub>3</sub> -LiTaO <sub>3</sub>	5a	Dielectric constant: Fig. 685.
Nr. 1C-e8 SrTiO <sub>3</sub> -Bi <sub>2</sub> O <sub>3</sub> · 3TiO <sub>2</sub>	1b	Lattice parameter: Fig. 686.
	5a	Dielectric constant: Fig. 687, 688.
Nr. 1C-e9 BaTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub>	1b	Phase diagram: Fig. 689.

Nr. 1C-e10 BaTiO <sub>3</sub> -BaTa <sub>2</sub> O <sub>6</sub>	1b	Lattice parameter: Fig. 690.
	5a	Dielectric constant: Fig. 691.
Nr. 1C-e11 BaTiO <sub>3</sub> -A <sub>2</sub> B <sub>2</sub> O <sub>7</sub>	1b	Curie temperature: Fig. 692.
	5a	Dielectric constant: Fig. 693 ... 697.
Nr. 1C-e12 PbZrO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>		
For the solid solution with PbNb <sub>2</sub> O <sub>6</sub> as an end material see 5B-8.		
	1b	Phase diagram: Fig. 698.
	4	Thermal expansion: Fig. 699.
	5	Dielectric constant: Fig. 700.
Nr. 1C-e13 PbZrO <sub>3</sub> -PbTa <sub>2</sub> O <sub>6</sub>	1b	Phase diagram: Fig. 701.
	4	Thermal expansion: see Fig. 699.
	5	Dielectric constant: Fig. 702.
Nr. 1C-f1 CaTiO <sub>3</sub> -SrTiO <sub>3</sub> -BaTiO <sub>3</sub>	1b	Phase diagram: Fig. 703.
Nr. 1C-f2 CaTiO <sub>3</sub> -BaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1b	Phase diagram: Fig. 704, 705. Curie temperature: Fig. 706.
	7a	Electromechanical properties: see Nr. 1A-8, 7a.
Nr. 1C-f3 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -PbO:SnO <sub>2</sub>	1b	Phase diagram: Fig. 707.
	8b	Elastic properties: Fig. 708, 709.
Nr. 1C-f4 PbTiO <sub>3</sub> -PbHfO <sub>3</sub> -PbO:SnO <sub>2</sub>	1b	Phase diagram: Fig. 710.
Nr. 1C-f5 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -LaFeO <sub>3</sub>	1b	Phase diagram: Fig. 711. Lattice parameters: Fig. 712.
	1b	Phase diagram: Fig. 713. Lattice parameters: Fig. 714.
Nr. 1C-f7 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1b	Phase diagram: Fig. 715. Lattice parameters: Fig. 716.
	7a	Electromechanical property: Fig. 717, 718.
Nr. 1C-f8 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1b	Lattice parameters: Fig. 719. Curie temperature: Fig. 720.
	7a	Electromechanical property: Fig. 721.
Nr. 1C-f9 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -ABO <sub>3</sub>	1b	Phase diagram: Fig. 722.
Nr. 1C-f10 PbTiO <sub>3</sub> -SrTiO <sub>3</sub> -LaMnO <sub>3</sub>	1b	Curie temperature: Fig. 723.
Nr. 1C-f11 PbTiO <sub>3</sub> -LaMnO <sub>3</sub> -LaMeO <sub>3</sub> (Me = Fe, Co, Ni, Cr)		
	1b	Transition temperatures: Fig. 724.
	5a	Dielectric constant: Fig. 725.
	11	Magnetic susceptibility: see Fig. 725. Magnetization: Fig. 726.

11 2 WO<sub>3</sub>

Nr. 1C-f12 BaTiO<sub>3</sub>-SrTiO<sub>3</sub>-LaYO<sub>3</sub>-LaInO<sub>3</sub>

1b | Phase diagram: Fig. 727.

Nr. 1C-f13 CaSnO<sub>3</sub>-SrSnO<sub>3</sub>-BaSnO<sub>3</sub>

1b | Phase diagram: Fig. 728.

Nr. 1C-f14 (Na-K)(Nb-Ta)O<sub>3</sub>

1b | Phase diagram: Fig. 729.

Nr. 1C-f15 (Ca-Ba)(Ti-Zr)O<sub>3</sub>

1b | Phase diagram: Fig. 730.

Nr. 1C-f16 (Sr-Pb)(Ti-Zr)O<sub>3</sub>

1b | Phase diagram: Fig. 731.  
Lattice parameter: Fig. 732.  
Transition temperature: Fig. 733.

5a | Dielectric constant: Fig. 734, 735.

Nr. 1C-f17 (Ba-Pb)(Ti-Zr)O<sub>3</sub>

1b | Phase diagram: Fig. 736.  
Lattice parameter: Fig. 737.  
Transition temperature: Fig. 738.

7a | Electromechanical properties: Fig. 739, 740.

Nr. 1C-f18 (Ba-Pb)(Ti-Sn)O<sub>3</sub>

1b | Phase diagram: Fig. 741, 742.  
Lattice parameter: Fig. 743.  
Transition temperature: Fig. 744.

Nr. 1C-f19 BaTiO<sub>3</sub>-PbTiO<sub>3</sub>-BaNb<sub>2</sub>O<sub>6</sub>-PbNb<sub>2</sub>O<sub>6</sub>

1b | Phase diagram: Fig. 745.  
Lattice parameter: Fig. 746.

2 WO<sub>3</sub>

2A Pure compound

Nr. 2A-1 WO<sub>3</sub>, Tungsten trioxide

1a	The anomalous dielectric properties of ceramic specimens of WO <sub>3</sub> were discovered by OGAWA <sup>a)</sup> in 1948. Possibility of ferroelectricity in WO <sub>3</sub> was pointed out by MATTHIAS <sup>b)</sup> in 1949.							
b	phase	VII	VI	V	IV	III	II	I
	state	F <sup>a)</sup>						
	crystal system	mono-clinic <sup>a)</sup>	tri-clinic <sup>b)</sup>	mono-clinic <sup>c)</sup>	ortho-rhombic <sup>b)</sup>	tetra-gonal <sup>d)</sup>	tetra-gonal <sup>b)</sup>	tetra-gonal <sup>b)</sup>
	space group			P2 <sub>1</sub> /n <sup>c)</sup> -C <sub>2h</sub> <sup>5)</sup>		P4/nmm <sup>d)</sup> -D <sub>2h</sub> <sup>7)</sup>		
	Θ	-40 <sup>b)</sup>	17 <sup>b)</sup>	330 <sup>e)</sup>	740 <sup>e)</sup>	910 <sup>e)</sup>	1230 <sup>e)</sup>	°C
	<i>T</i> <sub>melt</sub> = 1473 °C. <i>ρ</i> = 7.157 · 10 <sup>3</sup> kg m <sup>-3</sup> at RT. <i>a</i> = 7.30 Å, <i>b</i> = 7.53 Å, <i>c</i> = 7.68 Å, β = 90° 54' at 30 °C. Transparent, bluish green.							
2a	Crystal growth: Sublimation method.							
b	Crystal form: Plate-like.							
3	Crystal structure: Fig. 747, 748; Tab. 79; Fig. 749.							
	phase	VII	VI	V	IV	III	II	I
	Z	4	8	8				
4	Lattice distortion: Tab. 80. Thermal expansion: Fig. 750 ... 754.							
5a	Dielectric constant: κ = 100 ... 300 at liquid air temperature. No reliable dielectric measurements could be carried out at and above room temperature because of high electrical conductivity. <i>d</i> Θ <sub>IV-III</sub> / <i>d</i> <i>p</i> = -8.46 · 10 <sup>-8</sup> °K N <sup>-1</sup> m <sup>2</sup> .							
c	Dielectric hysteresis loop was observed at liquid air temperature.							

<sup>a)</sup> As to the crystal system in the phase VII, possibility of triclinic symmetry was discussed by TANISAKI [60T1].

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## V Index of substances — Substanzenverzeichnis

This index consists of two parts: part A is for pure compounds (including complex compounds such as  $\text{Pb}(\text{Co}_{1/2}\text{Nb}_{1/2})\text{O}_3$  or  $\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$ ) and part B is for solid solutions.

V A: In the 1st column the substances are ordered according to the alphabetically arranged gross formula. When their names (e.g. Rochelle salt) and/or their abbreviated names (e.g. TGS) are widely used, they are also included in this column. In the gross formula the numbers of the elements are determined by simple addition.

Compounds containing water of crystallization are, however, listed twice: (1) H and O of the water molecules are included in the gross formula, (2) the water molecules are attached separately to the gross formula. For instance, Rochelle salt is listed in the 1st column as  $\text{C}_4\text{H}_4\text{KNaO}_6 \cdot 4\text{H}_2\text{O}$ ,  $\text{C}_4\text{H}_{12}\text{KNaO}_{10}$  and also as Rochelle salt, RS, Seignette salt.

Crystals in which H is replaced by D (e.g.  $\text{KD}_2\text{PO}_4$ ) are not listed separately, since data on their properties are presented in the same section as the data on the non-deuterated crystals (e.g.  $\text{KH}_2\text{PO}_4$ ).

V B: In the 1st column the gross formula of each end material of a solid solution (e.g.  $\text{BaTiO}_3$  or  $\text{PbTiO}_3$  for the solid solution  $\text{BaTiO}_3$ - $\text{PbTiO}_3$ ) is listed in the same manner as in the case of pure compounds. Thus the solid solution  $\text{BaTiO}_3$ - $\text{PbTiO}_3$  can be found in the 2nd column by looking first for either  $\text{BaO}_3\text{Ti}$  or  $\text{O}_3\text{PbTi}$  in the 1st column of Part B. If the solid solution is expressed by the formula such as  $(\text{Sb}_x\text{Bi}_{1-x})\text{SI}$ , the end material can be obtained by putting  $x$  equal to either 0 or 1. When solid solutions have abbreviated names (e.g. KTN), these are also included in the 1st column.

Since in general one section corresponds to one substance in this volume, the 3rd column gives the section number and the 4th column gives the first page of the section.

Dieses Verzeichnis besteht aus zwei Teilen: Teil A enthält die reinen Verbindungen (einschließlich komplexer Verbindungen wie  $\text{Pb}(\text{Co}_{1/2}\text{Nb}_{1/2})\text{O}_3$  oder  $\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$ ) und Teil B enthält die Mischkristalle.

V A: In der 1. Spalte sind die Substanzen nach der alphabetisch angeordneten Bruttoformel aufgeführt. Wenn ihre Namen (z. B. Seignette-Salz) und/oder ihre abgekürzten Bezeichnungen (z. B. TGS) häufig gebraucht werden, sind auch sie in dieser Spalte zu finden. In der Bruttoformel ist die Anzahl jedes Elements durch einfache Addition bestimmt.

Verbindungen, die Kristallwasser enthalten, sind zweimal aufgeführt: 1. H und O der Wassermoleküle sind in der Bruttoformel enthalten. 2. die Wassermoleküle werden getrennt der Bruttoformel hinzugefügt (z. B. Seignette-Salz ist in der 1. Spalte aufgeführt als  $\text{C}_4\text{H}_4\text{KNaO}_6 \cdot 4\text{H}_2\text{O}$ ,  $\text{C}_4\text{H}_{12}\text{KNaO}_{10}$  und auch als Rochelle-Salz, RS, Seignette-Salz).

Kristalle, in denen H durch D ersetzt ist (z. B.  $\text{KD}_2\text{PO}_4$ ), werden nicht gesondert aufgeführt. Daten von ihren Eigenschaften erscheinen in demselben Abschnitt an der gleichen Stelle wie die Daten von den nicht deuterierten Kristallen (z. B.  $\text{KH}_2\text{PO}_4$ ).

V B: In der 1. Spalte ist die Bruttoformel jeder Endsubstanz einer Mischkristallreihe (z. B.  $\text{BaTiO}_3$  oder  $\text{PbTiO}_3$  für die Mischkristallreihe  $\text{BaTiO}_3$ - $\text{PbTiO}_3$ ) in derselben Weise aufgeführt wie im Fall von reinen Verbindungen. So kann die Mischkristallreihe  $\text{BaTiO}_3$ - $\text{PbTiO}_3$  in der zweiten Spalte gefunden werden, wenn man zunächst entweder  $\text{BaO}_3\text{Ti}$  oder  $\text{O}_3\text{PbTi}$  in der ersten Spalte von Teil B sucht. Wenn die Mischkristallreihe durch die Formel  $(\text{Sb}_x\text{Bi}_{1-x})\text{SI}$  ausgedrückt wird, kann man die Endsubstanz finden, indem man  $x$  gleich 0 oder 1 setzt. Wenn Mischkristalle abgekürzte Namen haben (z. B. KTN), sind diese auch in der 1. Spalte enthalten.

Da in diesem Band jeweils ein Abschnitt einer Substanz entspricht, gibt die 3. Spalte die Abschnittsnummer und die 4. Spalte die erste Seite des Abschnitts an.

## VA Pure compounds

Gross formula	Chemical formula	Nr.	Page
ADP	$\text{NH}_4\text{H}_2\text{PO}_4$	13A-7	143
$\text{AgC}_2\text{H}_3\text{N}_2\text{O}_5$	$\text{NH}_2\text{CH}_2\text{COOH} \cdot \text{AgNO}_3$	29A-1	191
$\text{Ag}_2\text{H}_3\text{IO}_6$	$\text{Ag}_2\text{H}_3\text{IO}_6$	35-22	209
$\text{AgNbO}_3$	$\text{AgNbO}_3$	35-16	207
$\text{AgO}_3\text{Ta}$	$\text{AgTaO}_3$	35-18	207
$\text{AgO}_3\text{V}$	$\text{AgVO}_3$	35-20	208
$\text{AlCH}_6\text{NO}_8\text{S}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_2\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-4	158
$\text{AlCH}_6\text{N}_3\text{O}_8\text{S}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-1	161
$\text{AlCH}_{18}\text{N}_9\text{O}_{14}\text{S}_2$	$\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-1	161
$\text{AlCH}_{30}\text{NO}_{20}\text{S}_2$	$\text{CH}_3\text{NH}_2\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-4	158
$\text{AlCH}_6\text{NO}_8\text{Se}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_2\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-10	161
$\text{AlCH}_6\text{N}_3\text{O}_8\text{Se}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_2)_3\text{Al}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-5	166
$\text{AlCH}_{18}\text{N}_9\text{O}_{14}\text{Se}_2$	$\text{C}(\text{NH}_2)_3\text{Al}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-5	166
$\text{AlCH}_{30}\text{NO}_{20}\text{Se}_2$	$\text{CH}_3\text{NH}_2\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-10	161
Ammonium metaphosphate			
$\text{AsCsH}_2\text{O}_4$	$\text{CsH}_2\text{AsO}_4$	35-14	205
$\text{AsH}_2\text{KO}_4$	$\text{KH}_2\text{AsO}_4$	13A-6	143
		13A-4	141

## V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
AsH <sub>6</sub> NO <sub>4</sub>	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	13A-8	147
AsH <sub>2</sub> O <sub>4</sub> Rb	RbH <sub>2</sub> AsO <sub>4</sub>	13A-5	143
Azobenzene	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	37-5	216
Azoxybenzene	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O	37-6	216
B <sub>7</sub> BrCd <sub>3</sub> O <sub>13</sub>	Cd <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-18	120
B <sub>7</sub> BrCo <sub>3</sub> O <sub>13</sub>	Co <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-14	119
B <sub>7</sub> BrCr <sub>3</sub> O <sub>13</sub>	Cr <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-11	118
B <sub>7</sub> BrCu <sub>3</sub> O <sub>13</sub>	Cu <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-16	119
B <sub>7</sub> BrFe <sub>3</sub> O <sub>13</sub>	Fe <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-13	119
B <sub>7</sub> BrMg <sub>3</sub> O <sub>13</sub>	Mg <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-10	118
B <sub>7</sub> BrMn <sub>3</sub> O <sub>13</sub>	Mn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-12	119
B <sub>7</sub> BrNi <sub>3</sub> O <sub>13</sub>	Ni <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-15	119
B <sub>7</sub> BrO <sub>13</sub> Zn <sub>3</sub>	Zn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-17	120
B <sub>6</sub> Ca <sub>2</sub> H <sub>10</sub> O <sub>16</sub>	Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> · 5H <sub>2</sub> O	21A-1	173
B <sub>6</sub> Ca <sub>2</sub> O <sub>11</sub> · 5H <sub>2</sub> O	Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> · 5H <sub>2</sub> O	21A-1	173
B <sub>7</sub> Cd <sub>3</sub> ClO <sub>13</sub>	Cd <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-9	118
B <sub>7</sub> Cd <sub>3</sub> IO <sub>13</sub>	Cd <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-25	122
B <sub>7</sub> ClCo <sub>3</sub> O <sub>13</sub>	Co <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-5	117
B <sub>7</sub> ClCr <sub>3</sub> O <sub>13</sub>	Cr <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-2	116
B <sub>7</sub> ClCu <sub>3</sub> O <sub>13</sub>	Cu <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-7	118
B <sub>7</sub> ClFe <sub>3</sub> O <sub>13</sub>	Fe <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-4	117
B <sub>7</sub> ClMg <sub>3</sub> O <sub>13</sub>	Mg <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-1	115
B <sub>7</sub> ClMn <sub>3</sub> O <sub>13</sub>	Mn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-3	117
B <sub>7</sub> ClNi <sub>3</sub> O <sub>13</sub>	Ni <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-6	117
B <sub>7</sub> ClO <sub>13</sub> Zn <sub>3</sub>	Zn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-8	118
B <sub>7</sub> Co <sub>3</sub> IO <sub>13</sub>	Co <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-22	121
B <sub>7</sub> Cr <sub>3</sub> IO <sub>13</sub>	Cr <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-19	120
B <sub>7</sub> Fe <sub>3</sub> IO <sub>13</sub>	Fe <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-21	120
B <sub>7</sub> IMn <sub>3</sub> O <sub>13</sub>	Mn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-20	120
B <sub>7</sub> INi <sub>3</sub> O <sub>13</sub>	Ni <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-23	121
B <sub>7</sub> IO <sub>13</sub> Zn <sub>3</sub>	Zn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-24	121
Ba <sub>4</sub> Bi <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	Ba <sub>4</sub> Bi <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g1	104
BaBi <sub>2</sub> Nb <sub>8</sub> O <sub>9</sub>	BaBi <sub>2</sub> Nb <sub>8</sub> O <sub>9</sub>	7A-7	109
BaBi <sub>3</sub> NbO <sub>12</sub> Ti <sub>2</sub>	BaBi <sub>3</sub> Ti <sub>2</sub> NbO <sub>12</sub>	7A-12	110
BaBi <sub>2</sub> O <sub>9</sub> Ta <sub>2</sub>	BaBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub>	7A-8	109
BaBi <sub>4</sub> O <sub>15</sub> Ti <sub>4</sub>	BaBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	7A-14	111
Ba <sub>2</sub> Bi <sub>4</sub> O <sub>18</sub> Ti <sub>5</sub>	Ba <sub>2</sub> Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub>	7A-19	112
BaC <sub>18</sub> Ca <sub>2</sub> H <sub>30</sub> O <sub>12</sub>	Ca <sub>2</sub> Ba(CH <sub>2</sub> CH <sub>2</sub> COO) <sub>6</sub>	26A-3	184
Ba <sub>4</sub> Ce <sub>2</sub> Nb <sub>8</sub> Ni <sub>2</sub> O <sub>30</sub>	Ba <sub>4</sub> Ce <sub>2</sub> Ni <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-d1	104
Ba <sub>4</sub> Fe <sub>2</sub> Gd <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	Ba <sub>4</sub> Gd <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g4	104
Ba <sub>2</sub> Fe <sub>3</sub> Nb <sub>7</sub> Nd <sub>4</sub> O <sub>30</sub>	Ba <sub>2</sub> Nd <sub>4</sub> Fe <sub>3</sub> Nb <sub>7</sub> O <sub>30</sub>	5C-h1	104
Ba <sub>4</sub> Fe <sub>2</sub> Nb <sub>8</sub> Nd <sub>2</sub> O <sub>30</sub>	Ba <sub>4</sub> Nd <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g2	104
Ba <sub>4</sub> FeNb <sub>8</sub> O <sub>30</sub>	Ba <sub>4</sub> FeNb <sub>8</sub> O <sub>30</sub>	5C-f1	104
Ba <sub>2</sub> Fe <sub>3</sub> Nb <sub>7</sub> O <sub>30</sub> Sm <sub>4</sub>	Ba <sub>2</sub> Sm <sub>4</sub> Fe <sub>3</sub> Nb <sub>7</sub> O <sub>30</sub>	5C-h2	104
Ba <sub>4</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub> Sm <sub>2</sub>	Ba <sub>4</sub> Sm <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g3	104
Ba <sub>2</sub> KNb <sub>5</sub> O <sub>15</sub>	KBa <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b3	103
Ba <sub>9</sub> MgNb <sub>14</sub> O <sub>45</sub>	Ba <sub>9</sub> MgNb <sub>14</sub> O <sub>45</sub>	5C-e1	104
Ba <sub>2</sub> NaNb <sub>5</sub> O <sub>15</sub>	NaBa <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b2	103
Ba <sub>2</sub> Nb <sub>8</sub> Nd <sub>4</sub> Ni <sub>2</sub> O <sub>30</sub>	Ba <sub>2</sub> Nd <sub>4</sub> Ni <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-c1	104
Ba <sub>2</sub> Nb <sub>8</sub> Ni <sub>2</sub> O <sub>30</sub> Sm <sub>4</sub>	Ba <sub>2</sub> Sm <sub>4</sub> Ni <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-c2	104
Ba <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub> Rb	RbBa <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b5	103
Ba <sub>6</sub> Nb <sub>8</sub> O <sub>30</sub> Ti <sub>2</sub>	Ba <sub>6</sub> Ti <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-j1	104
BaNb <sub>1.5</sub> O <sub>5.25</sub> Zr <sub>0.25</sub>	BaZr <sub>0.25</sub> Nb <sub>1.5</sub> O <sub>5.25</sub>	5C-j3	105
BaO <sub>6</sub> Ta <sub>2</sub>	BaTa <sub>2</sub> O <sub>6</sub>	5A-3	98
BaO <sub>3</sub> Ti	BaTiO <sub>3</sub>	1A-8	51
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub>	1A-12	61
BeC <sub>6</sub> F <sub>4</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub>	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> H <sub>2</sub> BeF <sub>4</sub>	28A-3	190
BeF <sub>4</sub> H <sub>8</sub> N <sub>2</sub>	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>	14A-2	154
BiBrS	BiSBr	10A-7	126
BiBrSe	BiSeBr	10A-10	127
Bi <sub>2</sub> CaNb <sub>2</sub> O <sub>9</sub>	CaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	7A-3	107
Bi <sub>2</sub> CaO <sub>9</sub> Ta <sub>2</sub>	CaBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub>	7A-4	108
Bi <sub>4</sub> CaO <sub>15</sub> Ti <sub>4</sub>	CaBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	7A-17	112

## V Index of substances

Gross formula	Chemical formula	Nr.	Page
BiClS	BiSCl	10A-6	125
BiClSe	BiSeCl	10A-9	126
$\text{Bi}_2\text{Fe}_4\text{Nb}_6\text{Nd}_4\text{O}_{30}$	$\text{Bi}_2\text{Nd}_4\text{Fe}_4\text{Nb}_6\text{O}_{30}$	5C-i2	104
$\text{BiFeO}_3$	$\text{BiFeO}_3$	1A-15	63
$\text{Bi}_5\text{GaO}_{15}\text{Ti}_3$	$\text{BiBi}_4\text{Ti}_3\text{GaO}_{15}$	7A-18	112
BiIS	BiSI	10A-8	126
BiISe	BiSeI	10A-11	127
$\text{BiK}_2\text{Nb}_5\text{O}_{15}$	$\text{K}_2\text{BiNb}_5\text{O}_{15}$	5C-a2	102
$\text{Bi}_{1/2}\text{K}_{1/2}\text{O}_3\text{Ti}$	$(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1B1-i	64
$\text{Bi}_{4.5}\text{K}_{0.5}\text{O}_{15}\text{Ti}_4$	$\text{K}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$	7B-4	114
$\text{Bi}_{1/2}\text{Na}_{1/2}\text{O}_3\text{Ti}$	$(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1B1-ii	64
$\text{Bi}_{4.5}\text{Na}_{0.5}\text{O}_{15}\text{Ti}_4$	$\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$	7B-3	114
$\text{Bi}_2\text{Nb}_2\text{O}_9\text{Pb}$	$\text{PbBi}_2\text{Nb}_2\text{O}_9$	7A-9	109
$\text{Bi}_3\text{NbO}_{15}\text{PbTi}_2$	$\text{PbBi}_3\text{Ti}_2\text{NbO}_{12}$	7A-13	110
$\text{Bi}_2\text{Nb}_2\text{O}_9\text{Sr}$	$\text{SrBi}_2\text{Nb}_2\text{O}_9$	7A-5	108
$\text{Bi}_3\text{NbO}_9\text{Ti}$	$\text{BiBi}_2\text{TiNbO}_9$	7A-1	107
$\text{Bi}_2\text{O}_9\text{PbTa}_2$	$\text{PbBi}_2\text{Ta}_2\text{O}_9$	7A-10	110
$\text{Bi}_4\text{O}_{15}\text{PbTi}_4$	$\text{PbBi}_4\text{Ti}_4\text{O}_{15}$	7A-15	111
$\text{Bi}_4\text{O}_{18}\text{Pb}_2\text{Ti}_5$	$\text{Pb}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$	7A-20	112
$\text{Bi}_2\text{O}_9\text{SrTa}_2$	$\text{SrBi}_2\text{Ta}_2\text{O}_9$	7A-6	109
$\text{Bi}_4\text{O}_{18}\text{SrTi}_4$	$\text{SrBi}_4\text{Ti}_4\text{O}_{18}$	7A-16	111
$\text{Bi}_4\text{O}_{18}\text{Sr}_2\text{Ti}_5$	$\text{Sr}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$	7A-21	113
$\text{Bi}_3\text{O}_9\text{TaTi}$	$\text{BiBi}_2\text{TiTaO}_9$	7A-2	107
$\text{Bi}_2\text{O}_{11}\text{Ti}_4$	$\text{Bi}_2\text{Ti}_4\text{O}_{11}$	7A-22	113
$\text{Bi}_4\text{O}_{12}\text{Ti}_3$	$\text{BiBi}_2\text{Ti}_2\text{TiO}_{12}$	7A-11	110
$\text{Br}_3\text{C}_4\text{H}_{12}\text{HgN}$	$\text{N}(\text{CH}_3)_4\text{HgBr}_3$	24A-2	179
$\text{Br}_3\text{C}_4\text{H}_{12}\text{HgP}$	$\text{P}(\text{CH}_3)_4\text{HgBr}_3$	24A-3	180
BrH	H · Br	35-12	203
BrSSb	SbSBr	10A-1	122
BrSbSe	SbSeBr	10A-3	124
$\text{C}_9\text{CaCl}_2\text{H}_{21}\text{N}_3\text{O}_6$	$(\text{CH}_3\text{NHCH}_2\text{COOH})_3 \cdot \text{CaCl}_2$	32A-1	192
$\text{C}_{18}\text{Ca}_2\text{H}_{30}\text{O}_{12}\text{Pb}$	$\text{Ca}_2\text{Pb}(\text{CH}_2\text{CH}_2\text{COO})_6$	26A-2	183
$\text{C}_{18}\text{Ca}_2\text{H}_{30}\text{O}_{12}\text{Sr}$	$\text{Ca}_2\text{Sr}(\text{CH}_2\text{CH}_2\text{COO})_6$	26A-1	182
$\text{C}_4\text{Cl}_3\text{H}_{12}\text{HgN}$	$\text{N}(\text{CH}_3)_4 \cdot \text{HgCl}_3$	24A-1	178
$\text{C}_4\text{Cl}_3\text{H}_{10}\text{MnN}_3\text{O}_4 \cdot 2\text{H}_2\text{O}$	$(\text{NH}_2\text{CH}_2\text{COOH})_2 \cdot \text{MnCl}_2 \cdot 2\text{H}_2\text{O}$	31A-1	192
$\text{C}_4\text{Cl}_3\text{H}_{14}\text{MnN}_3\text{O}_6$	$(\text{NH}_2\text{CH}_2\text{COOH})_2 \cdot \text{MnCl}_2 \cdot 2\text{H}_2\text{O}$	31A-1	192
$\text{C}_2\text{ClH}_6\text{NO}_2$	$\text{CH}_2\text{ClCOONH}_4$	27A-1	184
$\text{C}_4\text{Cl}_2\text{H}_8\text{NO}_4$	$(\text{CH}_2\text{ClCOO})_2\text{H} \cdot \text{NH}_4$	27A-2	184
$\text{CCrH}_6\text{NO}_8\text{S}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_3\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-6	160
$\text{CCrH}_6\text{N}_3\text{O}_8\text{S}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_2)_3\text{Cr}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-2	164
$\text{CCrH}_{30}\text{NO}_{20}\text{S}_2$	$\text{CH}_3\text{NH}_3\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-6	160
$\text{CCrH}_{18}\text{N}_3\text{O}_{14}\text{S}_2$	$\text{C}(\text{NH}_2)_3\text{Cr}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-2	164
$\text{CCrH}_6\text{N}_3\text{O}_8\text{Se}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_2)_3\text{Cr}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-6	167
$\text{CCrH}_{18}\text{N}_3\text{O}_{14}\text{Se}_2$	$\text{C}(\text{NH}_2)_3\text{Cr}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-6	167
$\text{C}_2\text{CuH}_2\text{O}_4 \cdot 4\text{H}_2\text{O}$	$\text{Cu}(\text{HCOO})_2 \cdot 4\text{H}_2\text{O}$	25A-1	180
$\text{C}_2\text{CuH}_{10}\text{O}_8$	$\text{Cu}(\text{HCOO})_2 \cdot 4\text{H}_2\text{O}$	25A-1	180
$\text{C}_6\text{FeH}_6\text{K}_4\text{N}_6\text{O}_3$	$\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	22A-2	174
$\text{CFeH}_6\text{NO}_8\text{S}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_3\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-7	160
$\text{CFeH}_{30}\text{NO}_{20}\text{S}_2$	$\text{CH}_3\text{NH}_3\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-7	160
$\text{C}_6\text{FeK}_4\text{N}_6 \cdot 3\text{H}_2\text{O}$	$\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	22A-2	174
$\text{CGaH}_6\text{NO}_8\text{S}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_3\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-5	160
$\text{CGaH}_6\text{N}_3\text{O}_8\text{S}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_2)_3\text{Ga}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-3	165
$\text{CGaH}_{18}\text{N}_3\text{O}_{14}\text{S}_2$	$\text{C}(\text{NH}_2)_3\text{Ga}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-3	165
$\text{CGaH}_{30}\text{NO}_{20}\text{S}_2$	$\text{CH}_3\text{NH}_3\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-5	160
$\text{CGaH}_6\text{N}_3\text{O}_8\text{Se}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_2)_3\text{Ga}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-7	167
$\text{CGaH}_{18}\text{N}_3\text{O}_{14}\text{Se}_2$	$\text{C}(\text{NH}_2)_3\text{Ga}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-7	167
$\text{C}_4\text{H}_{12}\text{HgI}_3\text{N}$	$\text{N}(\text{CH}_3)_4\text{HgI}_3$	24A-4	180
$\text{C}_6\text{H}_6\text{K}_4\text{MnN}_6\text{O}_3$	$\text{K}_4\text{Mn}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	22A-1	174
$\text{C}_6\text{H}_6\text{K}_4\text{N}_6\text{O}_3\text{Os}$	$\text{K}_4\text{Os}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	22A-4	176
$\text{C}_6\text{H}_6\text{K}_4\text{N}_6\text{O}_3\text{Ru}$	$\text{K}_4\text{Ru}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	22A-3	176
$\text{C}_4\text{H}_4\text{KNaO}_6 \cdot 4\text{H}_2\text{O}$	$\text{NaKC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$	33A-1	193
$\text{C}_4\text{H}_{12}\text{KNaO}_{10}$	$\text{NaKC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$	33A-1	193
$\text{C}_4\text{H}_8\text{LiNO}_6 \cdot \text{H}_2\text{O}$	$\text{LiNH}_4 \cdot \text{C}_4\text{H}_4\text{O}_6 \cdot \text{H}_2\text{O}$	34A-1	199



## V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
$C_4H_{10}LiNO_7$	$LiNH_4 \cdot C_4H_4O_6 \cdot H_2O$	34A-1	199
$C_4H_4LiO_6Ti \cdot H_2O$	$LiTiC_4H_4O_6 \cdot H_2O$	34A-2	199
$C_4H_4LiO_6Ti$	$LiTiC_4H_4O_6 \cdot H_2O$	34A-2	199
$C_4H_8NNaO_6 \cdot 4H_2O$	$NaNH_4C_4H_4O_6 \cdot 4H_2O$	33A-2	197
$C_4H_8NNaO_{10}$	$NaNH_4C_4H_4O_6 \cdot 4H_2O$	33A-2	197
$C_4H_{11}N_3O_7$	$(NH_2CH_2COOH)_2 \cdot HNO_3$	30A-1	191
$C_6H_{17}N_3O_{10}S$	$(NH_2CH_2COOH)_3 \cdot H_2SO_4$	28A-1	185
$CH_6NO_8S_2V \cdot 12H_2O$	$CH_3NH_3V(SO_4)_2 \cdot 12H_2O$	18A-8	161
$CH_6N_3O_8S_2V \cdot 6H_2O$	$C(NH_2)_3V(SO_4)_2 \cdot 6H_2O$	19A-4	166
$CH_{18}N_3O_{14}S_2V$	$C(NH_2)_3V(SO_4)_2 \cdot 6H_2O$	19A-4	166
$CH_{30}NO_{20}S_2V$	$CH_3NH_3V(SO_4)_2 \cdot 12H_2O$	18A-8	161
$C_6H_{17}N_3O_{10}Se$	$(NH_2CH_2COOH)_3 \cdot H_2SeO_4$	28A-2	190
$CH_4N_2S$	$SC(NH_2)_2$	23A-1	177
$C_4H_8NaO_6Rb \cdot 4H_2O$	$NaRbC_4H_4O_6 \cdot 4H_2O$	33A-3	198
$C_4H_{12}NaO_{10}Rb$	$NaRbC_4H_4O_6 \cdot 4H_2O$	33A-3	198
$CH_6InNO_8S_2 \cdot 12H_2O$	$CH_3NH_3In(SO_4)_2 \cdot 12H_2O$	18A-9	161
$CH_{30}InNO_{20}S_2$	$CH_3NH_3In(SO_4)_2 \cdot 12H_2O$	18A-9	161
$C_6K_4MnN_6 \cdot 3H_2O$	$K_4Mn(CN)_6 \cdot 3H_2O$	22A-1	174
$C_6K_4N_6Os \cdot 3H_2O$	$K_4Os(CN)_6 \cdot 3H_2O$	22A-4	176
$C_6K_4N_6Ru \cdot 3H_2O$	$K_4Ru(CN)_6 \cdot 3H_2O$	22A-3	176
$CaO_3Ti$	$CaTiO_3$	1A-5	44
$CaO_3Zr$	$CaZrO_3$	1A-10	60
$Cd_2H_8N_2O_{12}S_3$	$(NH_4)_2Cd_2(SO_4)_3$	16A-1	156
$Cd_{1/4}Mn_{1/4}Nb_{1/2}O_3Pb$	$Pb(Cd_{1/4}Mn_{1/4}Nb_{1/2})O_3$	1B3-xvii	70
$Cd_{1/4}Mn_{1/4}O_3PbW_{1/2}$	$Pb(Cd_{1/4}Mn_{1/4}W_{1/2})O_3$	1B3-xvii	70
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7$	6A-1	105
$Cd_{1/3}Nb_{2/3}O_3Pb$	$Pb(Cd_{1/3}Nb_{2/3})O_3$	1B4-iii	71
$Cd_{1/2}O_3PbW_{1/2}$	$Pb(Cd_{1/2}W_{1/2})O_3$	1B2-ii	65
$CdO_3Ti$	$CdTiO_3$	1A-7	50
$Cl_3CsGe$	$CsGeCl_3$	35-21	208
$ClH$	$HCl$	35-11	202
$ClK$	$KCl$	35-28	211
$CoCrH_5N_3O_8S_2 \cdot 12H_2O$	$Co(NH_2)_2HCr(SO_4)_2 \cdot 12H_2O$	18A-11	161
$CoCrH_{23}N_3O_{20}S_2$	$Co(NH_2)_2HCr(SO_4)_2 \cdot 12H_2O$	18A-11	161
Colemanite	$Ca_2B_6O_{11} \cdot 5H_2O$ or $CaB_3O_4(OH)_3 \cdot H_2O$	21A-1	173
$Co_{1/4}Mn_{1/4}Nb_{1/2}O_3Pb$	$Pb(Co_{1/4}Mn_{1/4}Nb_{1/2})O_3$	1B3-xvii	70
$Co_{1/4}Mn_{1/4}O_3PbW_{1/2}$	$Pb(Co_{1/4}Mn_{1/4}W_{1/2})O_3$	1B3-xvii	70
$Co_{1/3}Nb_{2/3}O_3Pb$	$Pb(Co_{1/3}Nb_{2/3})O_3$	1B4-iv	71
$Co_{1/2}Nb_{1/2}O_3Pb$	$Pb(Co_{1/2}Nb_{1/2})O_3$	1B3-iv	68
$Co_{1/3}O_3PbTa_{2/3}$	$Pb(Co_{1/3}Ta_{2/3})O_3$	1B4-vii	72
$Co_{1/2}O_3PbTa_{1/2}$	$Pb(Co_{1/2}Ta_{1/2})O_3$	1B3-xiii	70
$Co_{1/2}O_3PbW_{1/2}$	$Pb(Co_{1/2}W_{1/2})O_3$	1B2-iv	66
$Cr_{1/4}Nb_{1/2}O_3PbSc_{1/4}$	$Pb(Sc_{1/4}Cr_{1/4}Nb_{1/2})O_3$	1B3-xvii	70
$CsH_2O_4P$	$CsH_2PO_4$	13A-3	141
$CsH_3O_6Se_2$	$CsH_3(SeO_3)_2$	20A-3	172
$CsNO_3$	$CsNO_3$	12A-3	134
Deoxyribonucleic acid	Deoxyribonucleic acid	35-33	212
DNA	Deoxyribonucleic acid	35-33	212
$ErMnO_3$	$ErMnO_3$	4A-2	95
$Eu_2Mo_3O_{12}$	$Eu_2(MoO_4)_3$	35-2	200
$F_7H_8N_2P$	$NH_4PF_6NH_4F$	35-24	210
$FeH_4NO_8S_2 \cdot 12H_2O$	$NH_4Fe(SO_4)_2 \cdot 12H_2O$	18A-1	157
$FeH_{28}NO_{20}S_2$	$NH_4Fe(SO_4)_2 \cdot 12H_2O$	18A-1	157
$Fe_4Nb_6Nd_6O_{30}$	$Nd_6Fe_4Nb_6O_{30}$	5C-i1	104
$Fe_3Nb_7Nd_4O_{30}Pb_2$	$Pb_2Nd_4Fe_3Nb_7O_{30}$	5C-h3	104
$Fe_{1/2}Nb_{1/2}O_3Pb$	$Pb(Fe_{1/2}Nb_{1/2})O_3$	1B3-iii	67
$FeNb_3O_{30}Sr_6$	$Sr_6FeNb_3O_{30}$	5C-f2	104
$Fe_2Nb_8O_{30}Sr_4Yb_2$	$Sr_4Yb_2Fe_2Nb_8O_{30}$	5C-g5	104
$Fe_{1/2}O_3PbTa_{1/2}$	$Pb(Fe_{1/2}Ta_{1/2})O_3$	1B3-xii	69
$Fe_{1/2}O_3PbW_{1/2}$	$Pb(Fe_{1/2}W_{1/2})O_3$	1B3-xvi	70
$Fe_{2/3}O_3PbW_{1/3}$	$Pb(Fe_{2/3}W_{1/3})O_3$	1B5-ii	73

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199	GASH	$C(NH_2)_3Al(SO_4)_2 \cdot 6H_2O$		
199	$Gd_2Mo_3O_{12}$	$Gd_2(MoO_4)_3$	19A-1	161
197	GeTe	GeTe	35-3	200
197	HI	HI	36-1	212
191	$H_{11}In_2O_6$	$(NH_4)_2H_3IO_6$	35-13	204
185	$H_4InNO_5S_2 \cdot 12H_2O$	$NH_4In(SO_4)_2 \cdot 12H_2O$	35-23	209
161	$H_{28}InNO_{20}S_2$	$NH_4In(SO_4)_2 \cdot 12H_2O$	18A-3	158
166	$H_2KO_4P$	$KH_2PO_4$	18A-3	158
166	$H_5LiN_2O_4S$	$Li(N_2H_5)SO_4$	13A-1	134
161	$H_3LiO_6Se_2$	$LiH_3(SeO_3)_2$	35-15	205
190	$H_4NNaO_4S \cdot 2H_2O$	$NaNH_4SO_4 \cdot 2H_2O$	20A-1	168
177	$H_8NNaO_5S$	$NaNH_4SO_4 \cdot 2H_2O$	17A-1	157
198	$H_6NO_4P$	$NH_4H_2PO_4$	17A-1	157
198	$H_5NO_4S$	$(NH_4)HSO_4$	13A-7	143
161	$H_5N_2O_4S$	$(NH_4)_2SO_4$	15A-1	154
161	$H_4NO_8S_2V \cdot 12H_2O$	$NH_4V(SO_4)_2 \cdot 12H_2O$	14A-1	148
174	$H_{28}NO_{20}S_2V$	$NH_4V(SO_4)_2 \cdot 12H_2O$	18A-2	158
176	$H_3NaO_6Se_2$	$NaH_3(SeO_3)_2$	18A-2	158
176	$H_2O$ (Ice)	$H_2O$	20A-2	169
44	$H_2O_4PRb$	$RbH_2PO_4$	35-29	211
60	$HO_4RbS$	$RbHSO_4$	13A-2	141
156	$HfO_3Pb$	$PbHfO_3$	15A-2	155
70	$HoMnO_3$	$HoMnO_3$	1A-14	62
70	$Ho_{1/2}Nb_{1/2}O_3Pb$	$Pb(Ho_{1/2}Nb_{1/2})O_3$	4A-3	95
105			1B3-viii	68
71	Ice	$H_2O$		
65	$IKO_3$	$KIO_3$	35-29	211
50	ISSb	$SbSI$	1A-16	64
208	ISbSe	$SbSeI$	10A-2	122
202	ISbTe	$SbTeI$	10A-4	125
211	$In_{1/2}Nb_{1/2}O_3Pb$	$Pb(In_{1/2}Nb_{1/2})O_3$	10A-5	125
161			1B3-vi	68
161	KDP	$KH_2PO_4$		
173	$K_2LaNb_5O_{15}$	$K_2LaNb_5O_{15}$	13A-1	134
70	$K_{0.6}Li_{0.4}NbO_3$	$K_{0.6}Li_{0.4}NbO_3$	5C-a1	102
70	$K_{0.6}Li_{0.4}Nb_{0.3}O_3Ta_{0.7}$	$K_{0.6}Li_{0.4}(Ta_{0.7}Nb_{0.3})O_3$	5C-k1	105
71	$KLiO_4S$	$KLiSO_4$	5C-k2	105
68	$KNO_2$	$KNO_2$	35-27	211
72	$KNO_3$	$KNO_3$	11A-2	130
70	$KNbO_3$	$KNbO_3$	12A-1	131
66	$KNb_5O_{15}Sr_2$	$KSr_2Nb_5O_{15}$	1A-2	39
70	$KO_3Ta$	$KTaO_3$	5C-b1	102
141			1A-4	41
172	Lecontite	$NaNH_4SO_4 \cdot 2H_2O$		
134	$LiNbO_3$	$LiNbO_3$	17A-1	157
212	$Li_{1/4}Nb_{1/4}O_3PbW_{1/2}$	$Pb(Li_{1/4}Nb_{1/4}W_{1/2})O_3$	3A-1	89
212	$LiO_3Ta$	$LiTaO_3$	1B3-xvii	70
	$LuMnO_3$	$LuMnO_3$	3A-2	92
95	$Lu_{1/2}Nb_{1/2}O_3Pb$	$Pb(Lu_{1/2}Nb_{1/2})O_3$	4A-6	97
200	$Lu_{1/2}O_3PbTa_{1/2}$	$Pb(Lu_{1/2}Ta_{1/2})O_3$	1B3-ix	68
			1B3-xv	70
210	MASD	$CH_3NH_3Al(SO_4)_2 \cdot 12H_2O$		
157	$Mg_{1/4}Mn_{1/4}Nb_{1/2}O_3Pb$	$Pb(Mg_{1/4}Mn_{1/4}Nb_{1/2})O_3$	18A-4	158
157	$Mg_{1/4}Mn_{1/4}O_3PbTa_{1/2}$	$Pb(Mg_{1/4}Mn_{1/4}Ta_{1/2})O_3$	1B3-xvii	70
104	$Mg_{1/4}Mn_{1/4}O_3PbW_{1/2}$	$Pb(Mg_{1/4}Mn_{1/4}W_{1/2})O_3$	1B3-xvii	70
104	$Mg_{1/3}Nb_{2/3}O_3Pb$	$Pb(Mg_{1/3}Nb_{2/3})O_3$	1B3-xvii	70
67	$MgNb_{14}O_{45}Sr_9$	$Sr_9MgNb_{14}O_{45}$	1B4-i	70
104	$Mg_{1/3}O_3PbTa_{2/3}$	$Pb(Mg_{1/3}Ta_{2/3})O_3$	5C-e2	104
104	$Mg_{1/2}O_3PbW_{1/2}$	$Pb(Mg_{1/2}W_{1/2})O_3$	1B4-vi	72
69	$Mn_{1/4}Nb_{1/2}Ni_{1/4}O_3Pb$	$Pb(Ni_{1/4}Mn_{1/4}Nb_{1/2})O_3$	1B2-i	65
70	$Mn_{1/2}Nb_{1/2}O_3Pb$	$Pb(Mn_{1/2}Nb_{1/2})O_3$	1B3-xvii	70
73	$Mn_{1/4}Nb_{1/2}O_3PbZn_{1/4}$	$Pb(Zn_{1/4}Mn_{1/4}Nb_{1/2})O_3$	1B3-ii	67
	$Mn_{1/4}Ni_{1/4}O_3PbW_{1/2}$	$Pb(Ni_{1/4}Mn_{1/4}W_{1/2})O_3$	1B3-xvii	70
			1B3-xvii	70

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MnO <sub>2</sub>	MnO <sub>2</sub>	35-31	212
Mn <sub>1/2</sub> O <sub>3</sub> PbRe <sub>1/2</sub>	Pb(Mn <sub>1/2</sub> Re <sub>1/2</sub> )O <sub>3</sub>	1B2-v	66
Mn <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Mn <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xi	69
Mn <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mn <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B2-iii	66
Mn <sub>2/3</sub> O <sub>3</sub> PbW <sub>1/3</sub>	Pb(Mn <sub>2/3</sub> W <sub>1/3</sub> )O <sub>3</sub>	1B5-i	73
MnO <sub>3</sub> Tm	TmMnO <sub>3</sub>	4A-4	96
MnO <sub>3</sub> Y	YMnO <sub>3</sub>	4A-1	94
MnO <sub>3</sub> Yb	YbMnO <sub>3</sub>	4A-5	96
Mo <sub>3</sub> O <sub>12</sub> Sm <sub>2</sub>	Sm <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-1	200
Mo <sub>3</sub> O <sub>12</sub> Tb <sub>2</sub>	Tb <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-4	201
NNaO <sub>2</sub>	NaNO <sub>2</sub>	11A-1	128
NO <sub>3</sub> Rb	RbNO <sub>3</sub>	12A-2	133
NaNbO <sub>3</sub>	NaNbO <sub>3</sub>	1A-1	37
NaO <sub>3</sub> Ta	NaTaO <sub>3</sub>	1A-3	40
NaO <sub>3</sub> V	NaVO <sub>3</sub>	35-19	208
Nb <sub>1/2</sub> Ni <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Ni <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-v	68
Nb <sub>2/3</sub> Ni <sub>1/3</sub> O <sub>3</sub> Pb	Pb(Ni <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B4-v	72
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub>	5A-1	97
Nb <sub>2</sub> O <sub>7</sub> Pb <sub>2</sub>	Pb <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6A-2	106
Nb <sub>1/2</sub> O <sub>3</sub> PbSc <sub>1/2</sub>	Pb(Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-i	67
Nb <sub>1/2</sub> O <sub>3</sub> PbYb <sub>1/2</sub>	Pb(Yb <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-vii	68
Nb <sub>2/3</sub> O <sub>3</sub> PbZn <sub>1/3</sub>	Pb(Zn <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B4-ii	71
Nb <sub>5</sub> O <sub>15</sub> RbSr <sub>2</sub>	RbSr <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b4	103
Ni <sub>1/3</sub> O <sub>3</sub> PbTa <sub>2/3</sub>	Pb(Ni <sub>1/3</sub> Ta <sub>2/3</sub> )O <sub>3</sub>	1B4-viii	73
O <sub>3</sub> PbSc <sub>1/2</sub> Ta <sub>1/2</sub>	Pb(Sc <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-x	69
O <sub>6</sub> Pb <sub>4</sub> Si	Pb <sub>4</sub> SiO <sub>6</sub>	35-26	210
O <sub>6</sub> PbTa <sub>2</sub>	PbTa <sub>2</sub> O <sub>6</sub>	5A-4	98
O <sub>3</sub> PbTa <sub>1/2</sub> Yb <sub>1/2</sub>	Pb(Yb <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xiv	70
O <sub>3</sub> PbTi	PbTiO <sub>3</sub>	1A-9	59
O <sub>6</sub> Pb <sub>3</sub> V <sub>2</sub>	Pb <sub>3</sub> V <sub>2</sub> O <sub>8</sub>	35-25	210
O <sub>3</sub> PbZr	PbZrO <sub>3</sub>	1A-13	61
O <sub>3</sub> RbTa	RbTaO <sub>3</sub>	35-17	207
O <sub>2</sub> Sn	SnO <sub>2</sub>	35-32	212
O <sub>6</sub> SrTa <sub>2</sub>	SrTa <sub>2</sub> O <sub>6</sub>	5A-2	98
O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub>	Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	6A-3	106
O <sub>3</sub> SrTi	SrTiO <sub>3</sub>	1A-6	45
O <sub>3</sub> SrZr	SrZrO <sub>3</sub>	1A-11	61
O <sub>2</sub> Ti	TiO <sub>2</sub>	35-30	212
O <sub>3</sub> W	WO <sub>3</sub>	2A-1	88
p-azoxyanisole	C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	37-1	215
p-azoxyphenetole	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	37-2	215
p-butoxybenzoic acid	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	37-3	215
Perovskite	CaTiO <sub>3</sub>	1A-5	44
p-methoxycinnamic acid	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>	37-4	216
Pyrolusite	MnO <sub>2</sub>	35-31	212
Rochelle salt	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
RS	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
Rutile	TiO <sub>2</sub>	35-30	212
Seignette salt	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
SiV <sub>3</sub>	V <sub>3</sub> Si	36-4	214
SnTe	SnTe	36-2	213
TGS	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> H <sub>2</sub> SO <sub>4</sub>	28A-1	185
Tri-glycine tellurate		28A-4	190

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212	ABO <sub>3</sub>	ABO <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>		
66	Al <sub>2</sub> BaO <sub>4</sub>	BaAl <sub>2</sub> O <sub>4</sub> -BaLi <sub>2</sub> F <sub>4</sub>	1C-f9	87
69	AlLaO <sub>3</sub>	LaAlO <sub>3</sub> -BaTiO <sub>3</sub>	8B-1	115
66	AlLaO <sub>3</sub>	LaAlO <sub>3</sub> -BiFeO <sub>3</sub>	1C-c8	83
73	AlLaO <sub>3</sub>	LaAlO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b11	83
96	AsH <sub>4</sub> NO <sub>4</sub>	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub> -TiH <sub>2</sub> AsO <sub>4</sub>	1C-c10	84
94	AsH <sub>2</sub> O <sub>4</sub> Ti	TiH <sub>2</sub> AsO <sub>4</sub> -NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	13B-3	148
200	AsIS	AsSI-SbSI	13B-3	148
201			10B-1	127
128	BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	(Ba-Pb)Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>		
133	BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	Bi <sub>2</sub> BaNb <sub>2</sub> O <sub>9</sub> -Bi <sub>2</sub> TiNbO <sub>9</sub>	7B-5	114
37	BaBi <sub>2</sub> NbO <sub>12</sub> Ti <sub>2</sub>	Bi <sub>2</sub> BaTi <sub>2</sub> NbO <sub>12</sub> -Bi <sub>2</sub> Ti <sub>2</sub> O <sub>12</sub>	7B-1	113
40	BaF <sub>4</sub> Li <sub>2</sub>	BaLi <sub>2</sub> F <sub>4</sub> -BaAl <sub>2</sub> O <sub>4</sub>	7B-2	113
208	BaFe <sub>1/2</sub> O <sub>3</sub> Ta <sub>1/2</sub>	Ba(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -BaTiO <sub>3</sub>	8B-1	115
68	BaHfO <sub>3</sub>	BaHfO <sub>3</sub> -BaTiO <sub>3</sub>	1C-d2	84
72	BaHfO <sub>3</sub>	BaHfO <sub>3</sub> -PbHfO <sub>3</sub>	1C-a24	77
97	BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub>	1C-a18	76
106	BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -BaZrO <sub>3</sub>	1C-e9	86
67	BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -CaNb <sub>2</sub> O <sub>6</sub>	5C-j2	105
68	BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-1	99
71	BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -SrNb <sub>2</sub> O <sub>6</sub>	5B-5	100
103	BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub> -PbTiO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-3	99
73	BaNb <sub>2</sub> O <sub>6</sub>	(Ba-Pb-Sr)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	1C-f19	88
69	BaO <sub>3</sub> Sn	(Ba-Pb-Ca)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	5B-15	102
210	BaO <sub>3</sub> Sn	BaZr <sub>0.25</sub> Nb <sub>1.5</sub> O <sub>5.25</sub>	5B-15	102
98	BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -BaTiO <sub>3</sub>	5C-j3	105
70	BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-a25	77
59	BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a21	76
210	BaO <sub>3</sub> Sn	(Ba-Pb)(Sn-Ti)O <sub>3</sub>	1C-b10	83
61	BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -SrSnO <sub>3</sub>	1C-f18	88
207	BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -CaSnO <sub>3</sub> -SrSnO <sub>3</sub>	1C-a20	76
212	BaO <sub>3</sub> Sn	BaTa <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub>	1C-f13	88
98	BaO <sub>6</sub> Ta <sub>2</sub>	(Ba-Pb-Ca)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	1C-e10	87
106	BaO <sub>6</sub> Ta <sub>2</sub>	(Ba-Pb-Sr)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	5B-15	102
45	BaO <sub>6</sub> Ta <sub>2</sub>	BaTiO <sub>3</sub> -Ba(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	5B-15	102
61	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BaHfO <sub>3</sub>	1C-d2	84
212	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub>	1C-a24	77
88	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BaSnO <sub>3</sub>	1C-e9	86
215	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BaTa <sub>2</sub> O <sub>6</sub>	1C-a25	77
215	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BaUO <sub>3</sub>	1C-e10	87
215	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BaZrO <sub>3</sub>	1C-a26	77
44	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -BiFeO <sub>3</sub>	1C-a23	77
216	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Bi <sub>2</sub> Ti <sub>2</sub> O <sub>12</sub>	1C-c9	84
212	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub>	7B-6	114
193	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Co <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	1C-a7	74
193	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Co <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
212	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-e11	87
193	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -KNbO <sub>3</sub>	1C-d3	84
214	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -LaAlO <sub>3</sub>	1C-c5	83
213	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Mn <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	1C-c8	83
185	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Mn <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
190	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -NaNbO <sub>3</sub>	1C-e11	87
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Ni <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	1C-c2	83
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -Ni <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-e11	87
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b4	82
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a11	75
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-b3	82
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a9	75
	BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f2	87
			1C-f1	87

## V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -LaInO <sub>3</sub> -LaYO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f12	88
BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -PbTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-f19	88
BaO <sub>3</sub> Ti	(Ba-Ca)(Ti-Zr)O <sub>3</sub>	1C-f15	88
BaO <sub>3</sub> Ti	(Ba-Pb)(Ti-Sn)O <sub>3</sub>	1C-f18	88
BaO <sub>3</sub> Ti	(Ba-Pb)(Ti-Zr)O <sub>3</sub>	1C-f17	88
BaO <sub>3</sub> U	BaUO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a26	77
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub>	5C-j2	105
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a23	77
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -CaZrO <sub>3</sub>	1C-a12	76
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b9	82
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a15	76
BaO <sub>3</sub> Zr	(Ba-Ca)(Zr-Ti)O <sub>3</sub>	1C-f15	88
BaO <sub>3</sub> Zr	(Ba-Pb)(Zr-Ti)O <sub>3</sub>	1C-f17	88
BaO <sub>3</sub> Zr	BaZr <sub>0.25</sub> Nb <sub>1.5</sub> O <sub>5.25</sub>	5C-j3	105
BeF <sub>4</sub> H <sub>8</sub> N <sub>2</sub>	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub> -(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	14B-1	154
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c9	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -LaAlO <sub>3</sub>	1C-b11	83
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -LaCrO <sub>3</sub>	1C-b12	83
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -LaFeO <sub>3</sub>	1C-a33	82
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1C-d23	85
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c13	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -PbZrO <sub>3</sub>	1C-c14	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -SrFeO <sub>3</sub>	1C-c16	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -Sr(Sn <sub>1/3</sub> Mn <sub>2/3</sub> )O <sub>3</sub>	1C-d22	85
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -SrSnO <sub>3</sub>	1C-c15	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -SrTiO <sub>3</sub>	1C-c7	83
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f6	87
Bi <sub>5</sub> GaO <sub>15</sub> Ti <sub>3</sub>	Bi <sub>5</sub> Ti <sub>3</sub> GaO <sub>15</sub> -Bi <sub>4</sub> PbTi <sub>4</sub> O <sub>15</sub>	7B-7	114
BiIS	BiSI-SbSI	10B-5	128
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -BaTiO <sub>3</sub>	1C-d3	84
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-d20	85
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d5	84
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Zr	(K <sub>1/2</sub> Bi <sub>1/2</sub> )ZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-d17	85
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-d20	85
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d4	84
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-d21	85
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Zr	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )ZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-d16	85
BiNbO <sub>6</sub>	Bi(Nb-Ti)O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-14	102
Bi <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub>	Bi <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-13	102
Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> Pb	Bi <sub>2</sub> PbNb <sub>2</sub> O <sub>9</sub> -Bi <sub>2</sub> TiNbO <sub>9</sub>	7B-1	113
Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> Pb	Bi <sub>2</sub> PbNb <sub>2</sub> O <sub>9</sub> -BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	7B-5	114
Bi <sub>3</sub> NbO <sub>12</sub> PbTi <sub>2</sub>	Bi <sub>3</sub> PbTi <sub>2</sub> NbO <sub>12</sub> -Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub>	7B-2	113
Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> Sr	Bi <sub>2</sub> SrNb <sub>2</sub> O <sub>9</sub> -Bi <sub>2</sub> TiNbO <sub>9</sub>	7B-1	113
Bi <sub>3</sub> NbO <sub>12</sub> SrTi <sub>2</sub>	Bi <sub>3</sub> SrTi <sub>2</sub> NbO <sub>12</sub> -Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub>	7B-2	113
Bi <sub>3</sub> NbO <sub>9</sub> Ti	Bi <sub>3</sub> TiNbO <sub>9</sub> -Bi <sub>2</sub> BaNb <sub>2</sub> O <sub>9</sub>	7B-1	113
Bi <sub>3</sub> NbO <sub>9</sub> Ti	Bi <sub>3</sub> TiNbO <sub>9</sub> -Bi <sub>2</sub> PbNb <sub>2</sub> O <sub>9</sub>	7B-1	113
Bi <sub>3</sub> NbO <sub>9</sub> Ti	Bi <sub>3</sub> TiNbO <sub>9</sub> -Bi <sub>2</sub> SrNb <sub>2</sub> O <sub>9</sub>	7B-1	113
Bi <sub>4</sub> O <sub>15</sub> PbTi <sub>4</sub>	Bi <sub>4</sub> PbTi <sub>4</sub> O <sub>15</sub> -Bi <sub>5</sub> Ti <sub>3</sub> GaO <sub>15</sub>	7B-7	114
BiO <sub>6</sub> Ti	Bi(Ti-Nb)O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-14	102
Bi <sub>2</sub> O <sub>9</sub> Ti <sub>3</sub>	Bi <sub>2</sub> O <sub>3</sub> · 3TiO <sub>2</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-14	102
Bi <sub>2</sub> O <sub>9</sub> Ti <sub>3</sub>	Bi <sub>2</sub> O <sub>3</sub> · 3TiO <sub>2</sub> -SrTiO <sub>3</sub>	1C-e8	86
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -BaTiO <sub>3</sub>	7B-6	114
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -Bi <sub>3</sub> BaTi <sub>2</sub> NbO <sub>12</sub>	7B-2	113
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -Bi <sub>3</sub> PbTi <sub>2</sub> NbO <sub>12</sub>	7B-2	113
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -Bi <sub>3</sub> SrTi <sub>2</sub> NbO <sub>12</sub>	7B-2	113
BrSSb	SbSBr-SbSI	10B-3	127
C <sub>6</sub> FH <sub>17</sub> N <sub>3</sub> O <sub>9</sub> P	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> PO <sub>3</sub> F- (NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SO <sub>4</sub>	28B-2	191
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-1	176
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-Rb <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-2	176
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-Tl <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-3	177
C <sub>6</sub> FeH <sub>16</sub> N <sub>10</sub> · 3H <sub>2</sub> O	(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-1	176
C <sub>6</sub> FeH <sub>22</sub> N <sub>10</sub> O <sub>3</sub>	(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-1	176

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$C_6FeH_6N_6O_3Rb_4$	$Rb_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-2	176
$C_6FeH_6N_6O_3Ti_4$	$Ti_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-3	177
$C_6FeK_4N_6 \cdot 3H_2O$	$K_4Fe(CN)_6 \cdot 3H_2O - (NH_4)_4Fe(CN)_6 \cdot 3H_2O$	22B-1	176
$C_6FeK_4N_6 \cdot 3H_2O$	$K_4Fe(CN)_6 \cdot 3H_2O - Rb_4Fe(CN)_6 \cdot 3H_2O$	22B-2	176
$C_6FeK_4N_6 \cdot 3H_2O$	$K_4Fe(CN)_6 \cdot 3H_2O - Ti_4Fe(CN)_6 \cdot 3H_2O$	22B-3	177
$C_6FeN_6Rb_4 \cdot 3H_2O$	$Rb_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-2	176
$C_6FeN_6Ti_4 \cdot 3H_2O$	$Ti_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-3	177
$C_4H_4KNaO_6 \cdot 4H_2O$	$NaKC_4H_4O_6 \cdot 4H_2O - NaNH_4C_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_4H_4KNaO_6 \cdot 4H_2O$	$NaKC_4H_4O_6 \cdot 4H_2O - NaTiC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$C_4H_{12}KNaO_{10}$	$NaKC_4H_4O_6 \cdot 4H_2O - NaNH_4C_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_4H_{12}KNaO_{10}$	$NaKC_4H_4O_6 \cdot 4H_2O - NaTiC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$C_4H_6NNaO_6 \cdot 4H_2O$	$NaNH_4C_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_4H_6NNaO_{10}$	$NaNH_4C_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_6H_{17}N_3O_{10}S$	$(NH_2CH_2COOH)_3 \cdot H_2SO_4 - (NH_2CH_2COOH)_3 \cdot H_2PO_3F$	28B-2	191
$C_6H_{17}N_3O_{10}S$	$(NH_2CH_2COOH)_3 \cdot H_2SO_4 - (NH_2CH_2COOH)_3 \cdot H_2SeO_4$	28B-1	191
$C_6H_{17}N_3O_{10}Se$	$(NH_2CH_2COOH)_3 \cdot H_2SeO_4 - (NH_2CH_2COOH)_3 \cdot H_2SO_4$	28B-1	191
$C_4H_4NaO_6Ti \cdot 4H_2O$	$NaTiC_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$C_4H_{12}NaO_{10}Ti$	$NaTiC_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$CaHfO_3$	$CaHfO_3 - PbHfO_3$	1C-a16	76
$CaNb_2O_6$	$CaNb_2O_6 - BaNb_2O_6$	5B-1	99
$CaNb_2O_6$	$CaNb_2O_6 - NaNbO_3$	1C-e3	86
$CaNb_2O_6$	$CaNb_2O_6 - PbNb_2O_6$	5B-2	99
$CaNb_2O_6$	$(Ca-Ba-Pb)(Nb-Ta)_2O_6$	5B-15	102
$Ca_2Nb_2O_7$	$Ca_2Nb_2O_7 - Cd_2Nb_2O_7$	6B-1	106
$CaO_3Sn$	$CaSnO_3 - PbTiO_3$	1C-b6	82
$CaO_3Sn$	$CaSnO_3 - SrSnO_3$	1C-a19	76
$CaO_3Sn$	$CaSnO_3 - SrSnO_3 - BaSnO_3$	1C-f13	88
$CaO_4Ta_2$	$(Ca-Ba-Pb)(Ta-Nb)_2O_6$	5B-15	102
$Ca_2O_7Ta_2$	$Ca_2Ta_2O_7 - Sr_2Ta_2O_7$	6B-6	106
$CaO_3Ti$	$CaTiO_3 - BaTiO_3$	1C-a7	74
$CaO_3Ti$	$CaTiO_3 - CaZrO_3$	1C-a22	76
$CaO_3Ti$	$CaTiO_3 - NaNbO_3$	1C-c1	83
$CaO_3Ti$	$CaTiO_3 - PbTiO_3$	1C-a8	75
$CaO_3Ti$	$CaTiO_3 - SrTiO_3$	1C-a6	74
$CaO_3Ti$	$CaTiO_3 - BaTiO_3 - PbTiO_3$	1C-f2	87
$CaO_3Ti$	$CaTiO_3 - BaTiO_3 - SrTiO_3$	1C-f1	87
$CaO_3Ti$	$(Ca-Ba)(Ti-Zr)O_3$	1C-f15	88
$CaO_3Zr$	$CaZrO_3 - BaZrO_3$	1C-a12	76
$CaO_3Zr$	$CaZrO_3 - CaTiO_3$	1C-a22	76
$CaO_3Zr$	$CaZrO_3 - PbTiO_3$	1C-b5	82
$CaO_3Zr$	$CaZrO_3 - PbZrO_3$	1C-a13	76
$CaO_3Zr$	$(Ca-Ba)(Zr-Ti)O_3$	1C-f15	88
$CdNb_2O_6$	$CdNb_2O_6 - NaNbO_3$	1C-e4	86
$CdNb_2O_6$	$CdNb_2O_6 - PbNb_2O_6$	5B-10	101
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Ca_2Nb_2O_7$	6B-1	106
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Cd_2Ta_2O_7$	6B-3	106
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Mg_2Nb_2O_7$	6B-4	106
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Pb_2Nb_2O_7$	6B-2	106
$Cd_2O_7Ta_2$	$Cd_2Ta_2O_7 - Cd_2Nb_2O_7$	6B-3	106
$CdO_3Ti$	$CdTiO_3 - LiNbO_3$	1C-e7	86
$CdO_3Ti$	$CdTiO_3 - LiTaO_3$	1C-e7	86
$Ce_{1/2}Li_{1/2}O_3Ti$	$(Li_{1/2}Ce_{1/2})TiO_3 - PbTiO_3$	1C-d8	85
$CoLaO_3$	$LaCoO_3 - PbTiO_3 - LaMnO_3$	1C-f11	87
$Co_2Nb_2O_7$	$Co_2Nb_2O_7 - BaTiO_3$	1C-e11	87
$Co_2O_7Ta_2$	$Co_2Ta_2O_7 - BaTiO_3$	1C-e11	87
$CrLaO_3$	$LaCrO_3 - BiFeO_3$	1C-b12	83
$CrLaO_3$	$LaCrO_3 - PbTiO_3 - LaMnO_3$	1C-f11	87
$CsNO_3$	$CsNO_3 - RbNO_3$	12B-4	134
$Eu_2Mo_3O_{12}$	$(Eu-Gd)_2(MoO_4)_3$	35-5	201
$Eu_2Mo_3O_{12}$	$(Eu-Tb)_2(MoO_4)_3$	35-6	201

## V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -BiFeO <sub>3</sub>	1C-a33	82
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c12	84
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f5	87
Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub> -BiFeO <sub>3</sub>	1C-d23	85
Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f8	87
Fe <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-d11	85
Fe <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -PbZrO <sub>3</sub>	1C-d15	85
FeO <sub>3</sub> Sr	SrFeO <sub>3</sub> -BiFeO <sub>3</sub>	1C-c16	84
Fe <sub>1/2</sub> O <sub>3</sub> SrTa <sub>1/2</sub>	Sr(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -SrTiO <sub>3</sub>	1C-d1	84
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Eu) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-5	201
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Nd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-8	202
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Tb) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-9	202
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Y) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-7	202
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	Gd <sub>2</sub> ((Mo-W)O <sub>4</sub> ) <sub>3</sub>	35-10	202
Gd <sub>2</sub> O <sub>12</sub> W <sub>3</sub>	Gd <sub>2</sub> ((W-Mo)O <sub>4</sub> ) <sub>3</sub>	35-10	202
GeTe	GeTe-SnTe	36-3	214
H <sub>2</sub> KO <sub>4</sub> P	KH <sub>2</sub> PO <sub>4</sub> -NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	13B-1	148
H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	NH <sub>4</sub> NO <sub>3</sub> -KNO <sub>3</sub>	12B-1	134
H <sub>6</sub> NO <sub>4</sub> P	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> -KH <sub>2</sub> PO <sub>4</sub>	13B-1	148
H <sub>6</sub> NO <sub>4</sub> P	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> -TiH <sub>2</sub> PO <sub>4</sub>	13B-2	148
H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> S	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> -(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>	14B-1	154
H <sub>2</sub> O <sub>4</sub> PTi	TiH <sub>2</sub> PO <sub>4</sub> -NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	13B-2	148
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -BaHfO <sub>3</sub>	1C-a18	76
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -CaHfO <sub>3</sub>	1C-a16	76
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -Pb(Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1C-d18	85
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a29	82
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a31	82
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -SrHfO <sub>3</sub>	1C-a17	76
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -PbTiO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-f4	87
HfO <sub>3</sub> Sr	SrHfO <sub>3</sub> -PbHfO <sub>3</sub>	1C-a17	76
IK	KI-KNO <sub>3</sub>	12B-3	134
IOSb	SbOI-SbSI	10B-2	127
ISSb	SbSI-AsSI	10B-1	127
ISSb	SbSI-BiSI	10B-5	128
ISSb	SbSI-SbOI	10B-2	127
ISSb	SbSI-SbSBr	10B-3	127
ISSb	SbSI-SbSeI	10B-4	128
ISbSe	SbSeI-SbSI	10B-4	128
InLaO <sub>3</sub>	LaInO <sub>3</sub> -BaTiO <sub>3</sub> -LaYO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f12	88
KNO <sub>3</sub>	KNO <sub>3</sub> -KI	12B-3	134
KNO <sub>3</sub>	KNO <sub>3</sub> -NH <sub>4</sub> NO <sub>3</sub>	12B-1	134
KNO <sub>3</sub>	KNO <sub>3</sub> -RbNO <sub>3</sub>	12B-2	134
KNbO <sub>3</sub>	KNbO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c5	83
KNbO <sub>3</sub>	KNbO <sub>3</sub> -KTaO <sub>3</sub>	1C-a4	74
KNbO <sub>3</sub>	KNbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-a1	73
KNbO <sub>3</sub>	KNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-11	101
KNbO <sub>3</sub>	KNbO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c6	83
KNbO <sub>3</sub>	KNbO <sub>3</sub> -SrNb <sub>2</sub> O <sub>6</sub>	5C-b6	103
KNbO <sub>3</sub>	(K-Na)(Nb-Ta)O <sub>3</sub>	1C-f14	88
KNbO <sub>3</sub>	K <sub>0.6</sub> Li <sub>0.4</sub> (Nb <sub>0.3</sub> Ta <sub>0.7</sub> )O <sub>3</sub>	5C-k2	105
KNbO <sub>3</sub>	K(Nb <sub>0.65</sub> Ta <sub>0.35</sub> )O <sub>3</sub> (KTN)	1C-a5	74
KO <sub>3</sub> Sb	KSbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-b2	82
KO <sub>3</sub> Ta	KTaO <sub>3</sub> -KNbO <sub>3</sub>	1C-a4	74
KO <sub>3</sub> Ta	KTaO <sub>3</sub> -NaNbO <sub>3</sub>	1C-b1	82
KO <sub>3</sub> Ta	K(Ta <sub>0.35</sub> Nb <sub>0.65</sub> )O <sub>3</sub> (KTN)	1C-a5	74
KO <sub>3</sub> Ta	(K-Na)(Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	1C-f14	88
KO <sub>3</sub> Ta	K <sub>0.6</sub> Li <sub>0.4</sub> (Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	5C-k2	105
KTN	K(Ta <sub>0.35</sub> Nb <sub>0.65</sub> )O <sub>3</sub>	1C-a5	74

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Page	Gross formula	Chemical formula	Nr.	Page
82	LaFeO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c12	84
84	La <sub>1/2</sub> Li <sub>1/2</sub> O <sub>3</sub> Ti	(Li <sub>1/2</sub> La <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d6	84
87	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c11	84
87	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaCoO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
85	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaCrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
87	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
85	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaNiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
85	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -PbTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f10	87
84	La <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> La <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d7	85
84	La <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub>	La <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-12	101
201	LaNiO <sub>3</sub>	LaNiO <sub>3</sub> -LaMnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
202	LaO <sub>3</sub> Y	LaYO <sub>3</sub> -BaTiO <sub>3</sub> -LaInO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f12	88
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -CdTiO <sub>3</sub>	1C-e7	86
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -LiTaO <sub>3</sub>	3B-1	94
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-e1	86
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-11	101
214	Li <sub>1/2</sub> Nd <sub>1/2</sub> O <sub>3</sub> Ti	Li <sub>0.4</sub> K <sub>0.6</sub> (Nb <sub>0.5</sub> Ta <sub>0.7</sub> )O <sub>3</sub>	5C-k2	105
148	LiO <sub>3</sub> Ta	(Li <sub>1/2</sub> Nd <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d9	85
134	LiO <sub>3</sub> Ta	LiTaO <sub>3</sub> -CdTiO <sub>3</sub>	1C-e7	86
148	LiO <sub>3</sub> Ta	LiTaO <sub>3</sub> -LiNbO <sub>3</sub>	3B-1	94
148		Li <sub>0.4</sub> K <sub>0.6</sub> (Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	5C-k2	105
148	Mg <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Mg <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-4	106
154	Mg <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> -Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1C-d19	85
148	Mg <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f7	87
76	Mg <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> -Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1C-d19	85
76	Mg <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-d10	85
85	Mn <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Mn <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-d13	85
82	Mn <sub>2/3</sub> O <sub>3</sub> Sn <sub>1/3</sub> Sr	Sr(Sn <sub>1/3</sub> Mn <sub>2/3</sub> )O <sub>3</sub> -BiFeO <sub>3</sub>	1C-d22	85
82	Mn <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Mn <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e11	87
76	Mn <sub>2</sub> O <sub>7</sub> Ta <sub>2</sub>	Mn <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e11	87
87	Mo <sub>3</sub> Nd <sub>2</sub> O <sub>12</sub>	(Nd-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-8	202
76	Mo <sub>3</sub> O <sub>12</sub> Tb <sub>2</sub>	(Tb-Eu) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-6	201
134	Mo <sub>3</sub> O <sub>12</sub> Tb <sub>2</sub>	(Tb-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-9	202
127	Mo <sub>3</sub> O <sub>12</sub> Y <sub>2</sub>	(Y-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-7	202
127	NO <sub>3</sub> Rb	RbNO <sub>3</sub> -CsNO <sub>3</sub>	12B-4	134
128	NO <sub>3</sub> Rb	RbNO <sub>3</sub> KNO <sub>3</sub>	12B-2	134
127	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c2	83
127	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -CaNb <sub>2</sub> O <sub>6</sub>	1C-e3	86
128	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -CaTiO <sub>3</sub>	1C-c1	83
128	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -CdNb <sub>2</sub> O <sub>6</sub>	1C-e4	86
88	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -KNbO <sub>3</sub>	1C-a1	73
134	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -KSbO <sub>3</sub>	1C-b2	82
134	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -KTaO <sub>3</sub>	1C-b1	82
134	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -LiNbO <sub>3</sub>	1C-e1	86
83	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -NaVO <sub>3</sub>	1C-e2	86
74	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -NaSbO <sub>3</sub>	1C-a3	74
73	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -NaTaO <sub>3</sub>	1C-a2	74
101	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-e6	86
83	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -PbTiO <sub>3</sub>	5B-11	101
103	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -PbZrO <sub>3</sub>	1C-c3	83
88	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -SrNb <sub>2</sub> O <sub>6</sub>	1C-c4	83
105	NaO <sub>3</sub> Sb	(Na-K)(Nb-Ta)O <sub>3</sub>	1C-e5	86
74	NaO <sub>3</sub> Ta	NaSbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-f14	88
82	NaO <sub>3</sub> Ta	NaTaO <sub>3</sub> -NaNbO <sub>3</sub>	1C-a3	74
74	NaO <sub>3</sub> V	(Na-K)(Ta-Nb)O <sub>3</sub>	1C-a2	74
82	Nb <sub>2</sub> Ni <sub>2</sub> O <sub>7</sub>	NaVO <sub>3</sub> -NaNbO <sub>3</sub>	1C-f14	88
74	Nb <sub>2</sub> O <sub>6</sub> Pb	Ni <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e2	86
88	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -BaNb <sub>2</sub> O <sub>6</sub>	1C-e11	87
105	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Bi <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub>	5B-5	100
74	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Bi <sub>2</sub> O <sub>3</sub> · 3TiO <sub>2</sub>	5B-13	102
		PbNb <sub>2</sub> O <sub>6</sub> -CaNb <sub>2</sub> O <sub>6</sub>	5B-14	102
			5B-2	99



## V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-CdNb}_2\text{O}_6$	5B-10	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-KNbO}_3$	5B-11	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-La}_2\text{O}_3 \cdot 3\text{Nb}_2\text{O}_5$	5B-12	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-LiNbO}_3$	5B-11	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-NaNbO}_3$	1C-e6,	86
$\text{Nb}_2\text{O}_6\text{Pb}$		5B-11	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-PbO : SnO}_2$	5B-9	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-PbTa}_2\text{O}_6$	5B-6	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-PbTiO}_3$	5B-7	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-PbZrO}_3$	5B-8,	101
$\text{Nb}_2\text{O}_6\text{Pb}$		1C-e12	87
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-RbNbO}_3$	5B-11	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-Sm}_2\text{O}_3 \cdot 3\text{Nb}_2\text{O}_5$	5B-12	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-SrNb}_2\text{O}_6$	5B-4	100
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-Y}_2\text{O}_3 \cdot 3\text{Nb}_2\text{O}_5$	5B-12	101
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-Bi(Nb-Ti)O}_6$	5B-14	102
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{PbNb}_2\text{O}_6\text{-BaNb}_2\text{O}_6\text{-BaTiO}_3\text{-PbTiO}_3$	1C-f19	88
$\text{Nb}_2\text{O}_6\text{Pb}$	$(\text{Pb-Ba-Ca})(\text{Nb-Ta})_2\text{O}_6$	5B-15	102
$\text{Nb}_2\text{O}_6\text{Pb}$	$(\text{Pb-Ba-Sr})(\text{Nb-Ta})_2\text{O}_6$	5B-15	102
$\text{Nb}_2\text{O}_6\text{Pb}$	$\text{Pb}_2\text{Nb}_2\text{O}_7\text{-Cd}_2\text{Nb}_2\text{O}_7$	6B-2	106
$\text{Nb}_{1/2}\text{O}_3\text{PbSc}_{1/2}$	$\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3\text{-PbHfO}_3$	1C-d18	85
$\text{Nb}_{1/2}\text{O}_3\text{PbSc}_{1/2}$	$\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3\text{-PbTiO}_3$	1C-d12	85
$\text{Nb}_{1/2}\text{O}_3\text{PbSc}_{1/2}$	$\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3\text{-PbZrO}_3$	1C-d14	85
$\text{NbO}_2\text{Rb}$	$\text{RbNbO}_3\text{-PbNb}_2\text{O}_6$	5B-11	101
$\text{Nb}_6\text{O}_{18}\text{Sm}_2$	$\text{Sm}_2\text{O}_3 \cdot 3\text{Nb}_2\text{O}_5\text{-PbNb}_2\text{O}_6$	5B-12	101
$\text{Nb}_2\text{O}_6\text{Sr}$	$\text{SrNb}_2\text{O}_6\text{-BaNb}_2\text{O}_6$	5B-3	99
$\text{Nb}_2\text{O}_6\text{Sr}$	$\text{SrNb}_2\text{O}_6\text{-KNbO}_3$	5C-b6	103
$\text{Nb}_2\text{O}_6\text{Sr}$	$\text{SrNb}_2\text{O}_6\text{-NaNbO}_3$	1C-e5	86
$\text{Nb}_2\text{O}_6\text{Sr}$	$\text{SrNb}_2\text{O}_6\text{-PbNb}_2\text{O}_6$	5B-4	100
$\text{Nb}_2\text{O}_6\text{Sr}$	$(\text{Sr-Ba-Pb})(\text{Nb-Ta})_2\text{O}_6$	5B-15	102
$\text{Nb}_2\text{O}_6\text{Sr}_2$	$\text{Sr}_2\text{Nb}_2\text{O}_7\text{-Sr}_2\text{Ta}_2\text{O}_7$	6B-5	106
$\text{Ni}_2\text{O}_7\text{Ta}_2$	$\text{Ni}_2\text{Ta}_2\text{O}_7\text{-BaTiO}_3$	1C-e11	87
$\text{Nb}_2\text{O}_{18}\text{Y}_2$	$\text{Y}_2\text{O}_3 \cdot 3\text{Nb}_2\text{O}_5\text{-PbNb}_2\text{O}_6$	5B-12	101
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-BaSnO}_3$	1C-a21	76
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-BaTiO}_3$	1C-b4	82
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-PbNb}_2\text{O}_6$	5B-9	101
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-PbTiO}_3$	1C-a30	82
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-PbZrO}_3$	1C-a32	82
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-PbHfO}_3\text{-PbTiO}_3$	1C-f4	87
$\text{O}_3\text{PbSn}$	$\text{PbO : SnO}_2\text{-PbTiO}_3\text{-PbZrO}_3$	1C-f3	87
$\text{O}_3\text{PbSn}$	$(\text{Pb-Ba})(\text{Sn-Ti})\text{O}_3$	1C-f18	88
$\text{O}_3\text{PbTa}_2$	$\text{PbTa}_2\text{O}_6\text{-PbNb}_2\text{O}_6$	5B-6	101
$\text{O}_3\text{PbTa}_2$	$\text{PbTa}_2\text{O}_6\text{-PbZrO}_3$	1C-e13	87
$\text{O}_3\text{PbTa}_2$	$\text{PbTa}_2\text{O}_6\text{-SrTa}_2\text{O}_6$	5B-16	102
$\text{O}_3\text{PbTa}_2$	$(\text{Pb-Ba-Ca})(\text{Ta-Nb})_2\text{O}_6$	5B-15	102
$\text{O}_3\text{PbTa}_2$	$(\text{Pb-Ba-Sr})(\text{Ta-Nb})_2\text{O}_6$	5B-15	102
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-BaSnO}_3$	1C-b10	83
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-BaTiO}_3$	1C-a11	75
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-BaZrO}_3$	1C-b9	82
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-BiFeO}_3$	1C-c13	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-CaSnO}_3$	1C-b6	82
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-CaTiO}_3$	1C-a8	75
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-CaZrO}_3$	1C-b5	82
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-(K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1C-d5	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-KNbO}_3$	1C-c6	83
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-LaAlO}_3$	1C-c10	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-LaFeO}_3$	1C-c12	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-LaMnO}_3$	1C-c11	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-(Li}_{1/2}\text{Ce}_{1/2})\text{TiO}_3$	1C-d8	85
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-(Li}_{1/2}\text{La}_{1/2})\text{TiO}_3$	1C-d6	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-(Li}_{1/2}\text{Nd}_{1/2})\text{TiO}_3$	1C-d9	85
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-(Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1C-d4	84
$\text{O}_3\text{PbTi}$	$\text{PbTiO}_3\text{-(Na}_{1/2}\text{La}_{1/2})\text{TiO}_3$	1C-d7	85

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Page	Gross formula	Chemical formula	Nr.	Page
101	$O_3PbTi$	$PbTiO_3-NaNbO_3$	1C-c3	83
101	$O_3PbTi$	$PbTiO_3-Pb(Fe_{1/2}Ta_{1/2})O_3$	1C-d11	85
101	$O_3PbTi$	$PbTiO_3-PbHfO_3$	1C-a29	82
101	$O_3PbTi$	$PbTiO_3-Pb(Mg_{1/2}W_{1/2})O_3$	1C-d10	85
86	$O_3PbTi$	$PbTiO_3-Pb(Mn_{1/2}Nb_{1/2})O_3$	1C-d13	85
101	$O_3PbTi$	$PbTiO_3-PbNb_2O_6$	5B-7	101
101	$O_3PbTi$	$PbTiO_3-PbO:SnO_2$	1C-a30	82
101	$O_3PbTi$	$PbTiO_3-Pb(Sc_{1/2}Nb_{1/2})O_3$	1C-d12	85
101	$O_3PbTi$	$PbTiO_3-PbZrO_3$	1C-a27	77
101	$O_3PbTi$	$PbTiO_3-SrSnO_3$	1C-b8	82
87	$O_3PbTi$	$PbTiO_3-SrTiO_3$	1C-a10	75
101	$O_3PbTi$	$PbTiO_3-SrZrO_3$	1C-b7	82
101	$O_3PbTi$	$PbTiO_3-ABO_3-PbZrO_3$	1C-f9	87
100	$O_3PbTi$	$PbTiO_3-BaTiO_3-CaTiO_3$	1C-f2	87
101	$O_3PbTi$	$PbTiO_3-BiFeO_3-PbZrO_3$	1C-f6	87
102	$O_3PbTi$	$PbTiO_3-LaCoO_3-LaMnO_3$	1C-f11	87
88	$O_3PbTi$	$PbTiO_3-LaCrO_3-LaMnO_3$	1C-f11	87
102	$O_3PbTi$	$PbTiO_3-LaFeO_3-LaMnO_3$	1C-f11	87
102	$O_3PbTi$	$PbTiO_3-LaFeO_3-PbZrO_3$	1C-f5	87
106	$O_3PbTi$	$PbTiO_3-LaMnO_3-LaNiO_3$	1C-f11	87
85	$O_3PbTi$	$PbTiO_3-LaMnO_3-SrTiO_3$	1C-f10	87
85	$O_3PbTi$	$PbTiO_3-Pb(Fe_{1/2}Nb_{1/2})O_3-PbZrO_3$	1C-f8	87
85	$O_3PbTi$	$PbTiO_3-PbHfO_3-PbO:SnO_2$	1C-f4	87
101	$O_3PbTi$	$PbTiO_3-Pb(Mg_{1/3}Nb_{2/3})O_3-PbZrO_3$	1C-f7	87
101	$O_3PbTi$	$PbTiO_3-PbO:SnO_2-PbZrO_3$	1C-f3	87
99	$O_3PbTi$	$PbTiO_3-BaTiO_3-BaNb_2O_6-PbNb_2O_6$	1C-f19	88
103	$O_3PbTi$	$(Pb-Ba)(Ti-Sn)O_3$	1C-f18	88
86	$O_3PbTi$	$(Pb-Ba)(Ti-Zr)O_3$	1C-f17	88
100	$O_3PbTi$	$Pb(Ti-Zr)O_3$	1C-a28	78
102	$O_3PbTi$	$(Pb-Sr)(Ti-Zr)O_3$	1C-f16	88
106	$O_3PbZr$	$PbZrO_3-BaTiO_3$	1C-b3	82
87	$O_3PbZr$	$PbZrO_3-BaZrO_3$	1C-a15	76
101	$O_3PbZr$	$PbZrO_3-BiFeO_3$	1C-c14	84
	$O_3PbZr$	$PbZrO_3-CaZrO_3$	1C-a13	76
76	$O_3PbZr$	$PbZrO_3-(K_{1/2}Bi_{1/2})ZrO_3$	1C-d17	85
82	$O_3PbZr$	$PbZrO_3-(Na_{1/2}Bi_{1/2})TiO_3$	1C-d21	85
101	$O_3PbZr$	$PbZrO_3-(Na_{1/2}Bi_{1/2})ZrO_3$	1C-d16	85
82	$O_3PbZr$	$PbZrO_3-NaNbO_3$	1C-c4	83
82	$O_3PbZr$	$PbZrO_3-Pb(Fe_{1/2}Ta_{1/2})O_3$	1C-d15	85
87	$O_3PbZr$	$PbZrO_3-PbHfO_3$	1C-a31	82
87	$O_3PbZr$	$PbZrO_3-PbNb_2O_6$	5B-8,	101
88			1C-e12	87
101	$O_3PbZr$	$PbZrO_3-PbO:SnO_2$	1C-a32	82
87	$O_3PbZr$	$PbZrO_3-Pb(Sc_{1/2}Nb_{1/2})O_3$	1C-d14	85
102	$O_3PbZr$	$PbZrO_3-PbTa_2O_6$	1C-e13	87
102	$O_3PbZr$	$PbZrO_3-PbTiO_3$	1C-a27	77
102	$O_3PbZr$	$PbZrO_3-SrZrO_3$	1C-a14	76
83	$O_3PbZr$	$Pb(Zr-Ti)O_3$ (PZT)	1C-a28	78
75	$O_3PbZr$	$PbZrO_3-ABO_3-PbTiO_3$	1C-f9	87
82	$O_3PbZr$	$PbZrO_3-BiFeO_3-PbTiO_3$	1C-f6	87
84	$O_3PbZr$	$PbZrO_3-LaFeO_3-PbTiO_3$	1C-f5	87
82	$O_3PbZr$	$PbZrO_3-Pb(Fe_{1/2}Nb_{1/2})O_3-PbTiO_3$	1C-f8	87
75	$O_3PbZr$	$PbZrO_3-Pb(Mg_{1/2}Nb_{1/2})O_3-PbTiO_3$	1C-f7	87
82	$O_3PbZr$	$PbZrO_3-PbO:SnO_2-PbTiO_3$	1C-f3	87
84	$O_3PbZr$	$(Pb-Ba)(Zr-Ti)O_3$	1C-f17	88
83	$O_3PbZr$	$(Pb-Sr)(Zr-Ti)O_3$	1C-f16	88
84	$O_3SnSr$	$SrSnO_3-BaSnO_3$	1C-a20	76
84	$O_3SnSr$	$SrSnO_3-BiFeO_3$	1C-c15	84
84	$O_3SnSr$	$SrSnO_3-CaSnO_3$	1C-a19	76
85	$O_3SnSr$	$SrSnO_3-PbTiO_3$	1C-b8	82
84	$O_3SnSr$	$SrSnO_3-BaSnO_3-CaSnO_3$	1C-f13	88
85	$O_6SrTa_2$	$SrTa_2O_6-PbTa_2O_6$	5B-16	102
84	$O_6SrTa_2$	$(Sr-Ba-Pb)(Ta-Nb)_2O_6$	5B-15	102
85	$O_7Sr_2Ta_2$	$Sr_2Ta_2O_7-Ca_2Ta_2O_7$	6B-6	106

## V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
$O_7Sr_2Ta_2$	$Sr_2Ta_2O_7-Sr_2Nb_2O_7$	6B-5	106
$O_3SrTi$	$SrTiO_3-BaTiO_3$	1C-a9	75
$O_3SrTi$	$SrTiO_3-BiFeO_3$	1C-c7	83
$O_3SrTi$	$SrTiO_3-Bi_2O_3 \cdot 3TiO_2$	1C-e8	86
$O_3SrTi$	$SrTiO_3-CaTiO_3$	1C-a6	74
$O_3SrTi$	$SrTiO_3-PbTiO_3$	1C-a10	75
$O_3SrTi$	$SrTiO_3-Sr(Fe_{1/2}Ta_{1/2})O_3$	1C-d1	84
$O_3SrTi$	$SrTiO_3-BaTiO_3-CaTiO_3$	1C-f1	87
$O_3SrTi$	$SrTiO_3-LaMnO_3-PbTiO_3$	1C-f10	87
$O_3SrTi$	$SrTiO_3-BaTiO_3-LaInO_3-LaYO_3$	1C-f12	88
$O_3SrZr$	$(Sr-Pb)(Ti-Zr)O_3$	1C-f16	88
$O_3SrZr$	$SrZrO_3-PbTiO_3$	1C-b7	82
$O_3SrZr$	$SrZrO_3-PbZrO_3$	1C-a14	76
$O_3SrZr$	$(Sr-Pb)(Zr-Ti)O_3$	1C-f16	88
PZT	$Pb(Zr-Ti)O_3$	1C-a28	78
SnTe	SnTe-GeTe	36-3	214

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